

MONITORING THE STATES OF SINGLE QUANTUM SYSTEMS

by

KEVIN GARAPO

Submitted in fulfilment of the academic requirements for the degree of Master of Science in the School of Chemistry and Physics, University of KwaZulu-Natal, Durban, South Africa.

April, 2012

As the candidates supervisor I have approved this dissertation for submission.

Signed: _____ Name: Thomas Konrad Date: ____ April, 2012.

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Abstract

Continuous weak measurement provide a convenient way to gather information about a quantum system without the need to prepare huge ensembles of identical systems as required by standard quantum measurement theory. Even though weak measurement alter the dynamics of the wave function slightly, they nevertheless are a good tool to monitor the dynamics of the wave function in real time in the presence of certain perturbations, for example, sudden momentum kicks due to collisions with particles of a surrounding gas. With weak measurement it is possible to monitor the dynamics of the wave function without knowing it initially. The continuous monitoring can be employed to influence the dynamics by means of feedback. This thesis focuses on the numeric simulation of the continuous monitoring of the position of a free massive particle as well as a particle bound in the following one-dimensional potentials: harmonic and double well. The monitoring scheme involves estimating the wave function of the hydrogen atom initially and then applying the results of the weak measurement its position to update the estimate through a numerically simulated stochastic evolution. We also simulate evolution of the true wave function. The key highlights of this thesis include: discussion of an alternative way to derive the stochastic differential equations that govern the evolution of the true and estimated wave functions of the system, as well as the explanation of the second order numerical scheme.

Preface

The work described in this thesis was carried out in the School University of KwaZulu-Natal, Durban, South Africa from February 2009 to April 2012, under the supervision of Professor Thomas Konrad and Professor Francesco Petruccione.

These studies represent original work by the author and have not otherwise been submitted in any form for any degree or diploma to any other tertiary institution. Where use has been made of the work of others it is duly acknowledged in the text.

Declaration 1 - Plagiarism

I, KEVIN GARAPO declare that

- a) The research reported in this thesis, except where otherwise indicated, is my original research.
- b) This thesis has not been submitted for any degree or examination at any other University.
- c) This thesis does not contain any other persons' data, pictures, graphs or other information unless specifically acknowledged as being sourced from other persons.
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 - (a) Their words have been re-written but the general information attributed to them has been referenced;
 - (b) Where their exact words have been used, their writing has been placed inside quotation marks, and references.
- e) This thesis does not contain text, graphics or tables copied and pasted from the Internet, unless specifically acknowledged, and the source being detailed in the thesis and the References sections.

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Publications

K. Garapo and T. Konrad. Alternative derivation of the master equation for a particle in an external field subject to continuous measurement. In *Proceedings of SAIP2011, the 56th annual conference of the South African Institute of Physics*, pages 780–785, 2011.

Signed: _____ Dated: ____ April, 2012.

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I would like to sincerely thank the National Research Foundation (NRF) for funding my research; and the University of KwaZulu-Natal, through the School of Physics, for providing excellent research facilities. I would also like to thank my colleagues and friends from the School of Physics for advising me, and providing moral support in times of great need. I regret the fact that the name-roll is so long, and that I cannot point out a few individuals without being unjust to others.

Lastly, I would like to pay homage to my family as well as the physics community in South Africa. My family has always supported me in every endeavour I have taken upon, this research being one of them. Whilst various physicists have sacrificed their time to provide stimulating advice and debate pertaining to various aspects of my research, which I presented at South African Institute of Physics conferences.

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Chapter 1

Introduction

The control of individual quantum systems promises a new technology for the twenty-first century - quantum technology.

—Howard M. Wiseman, Gerald J. Milburn [59]

Over the past few decades experimental advancements have made it possible to observe the dynamics of the state of an individual quantum system, such as an atom trapped by means of quantum cavity electrodynamics (QCED) [35, 17], or individual ions in cold traps [12, 54]. Individual quantum systems are the building blocks in quantum information processing, communication, and security. In fact, the unrivaled security offered by quantum-based cryptographic systems rely on the ability to encode information onto a quantum state [19, 7, 24, 6, 38, 36], which (in turn) is immune to cloning [60]; since performing a measurement on a quantum system disturbs its state, and a full state tomography requires a large ensemble of identical systems.

We will not dwell much on justifying the need for quantum technology, which evidently will play a significant role in information processing, and secure communication in the twenty-first century and beyond. However, we will take the liberty to highlight a few benefits of having such a technology. In the previous paragraph we highlighted the benefits of applying quantum theory to the problem of information security. Perhaps, it is imperative (at this moment) to point out that the advent of the quantum computer has been forecasted to greatly compromise the security of classically-encrypted information because most classical encryption algorithms rely heavily on computational complexity. One such, is the RSA [52] algorithm for public-key encryption, which relies on the complexity of factoring large integers. In 1994, Shor [56] showed that even though there exist no algorithms for the factorization of an integer in polynomial time on a classical Turing machine (universal computer), a quantum computer could solve the problem in polynomial time. This speed up implies that a quantum computer will be able to crack code, which a classical computer practically cannot, within an acceptable period of time; of course depending on the size of the problem. Fortunately,

there has been a lot of ground breaking work in the field of quantum cryptography and we can rest assured that we will still be able to secure our information even when the quantum computer becomes available.

This thesis presents the results of the numeric simulation of a method to monitor the position of a quantum system in real time. In order to achieve the monitoring of its state, the position of the system in question is measured continuously, but unsharply, and the measurement results are used to update its estimated wave function at each point in time. After some time the estimated state reasonably approximates the true state. Our notion of continuous measurement is that of a sequence of unsharp measurements performed at a high frequency, that is in the continuum limit. However, there is an upper bound as to how frequently one can observe the system without freezing the dynamics. This upper bound is a function of the Hamiltonian of the system, see [53]. The phenomenon in which repetitive observation a quantum system at high frequency inhibits unitary dynamics is called *quantum Zeno effect* [41, 27, 20]. So by striking a balance between the strength of measurement and the frequency of measurement, one can find a regime in which ample information can be extracted from the system to update the estimated wave function well enough to mimic the true wave function within an acceptable period of time. When this convergence takes place, the estimated wave function effectively represents the state of the system, and the corresponding evolution equation represents the dynamics. Empowered with this knowledge of the system, we have full control of it. This is in the sense that we can always apply a unitary operation to drive the state of the system into any other desired state.

This thesis consists of six chapters, and is written in the manner we shall describe shortly. Following this introductory chapter, we review the mathematical theory of measures in Chapter 2. Our main aim is to motivate the theory of quantum measurement from standard measure theory. This allows us to generalize the concept of measurement by representing measurements with Kraus operators [34] whose complete set of effects form positive operator-valued measures (POVM's). We then apply the concept of generalized measurement, in Chapter 3, to derive the master equations, and the corresponding stochastic Schrödinger equations for the evolution of the state of an individual quantum system, whose position is continuously observed. The work contained in this chapter has been published in the 2011 proceedings of the annual conference of the South African Institute of Physics [21]. Even though the derived equations for selective state evolution are the same as the ones that can be found in [14, 15], our approach differs from [14, 15] in that instead of re-deriving the Itô stochastic calculus (which was extensively done in [14]), we show an alternative way to derive the evolution equations from basic quantum mechanical principles, only applying stochastic calculus when required. This greatly simplifies the derivation. The way we derive the non-selective evolution equations, however, does not deviate from that of [32, 53]. We continue with this approach, in Chapter 4, and derive the evolution equations for the estimation of the state of the quantum system.

In Chapter 5 we review numerical simulation methods for stochastic differential equations. The aim of the chapter is to provide the necessary techniques to derive numerical integration schemes of desired orders of convergence, rather than restricting ourselves to a specific scheme. The theory presented in this chapter was not developed by us but rather compiled from the following sources [22, 30, 31, 49, 47, 40, 10, 45, 50, 53, 39, 9, 28, 46, 48]. The key concept is the application of Taylor-like expansions to stochastic differential equations in order to derive the various numerical integration schemes. It is important to point out that Itô calculus was extensively used. However, we stuck with the philosophy of keeping the presentation as simple and straight-forward as possible. We go on to show the results of numeric simulations in this chapter.

Chapter 2

Generalized Measurements

2.1 Introduction

The projection postulate, which prescribes “collapse of the state vector” upon measurement, is not an essential part of quantum mechanics. Rather it is only an optional discarding of certain branches of the state vector that are expected to be irrelevant for the purpose at hand. However, its use is hazardous, and there are examples of repeated measurements for which the conventional application of the projection postulate leads to incorrect results.

–L. E. Ballentine [4]

The above statements by Ballentine sum up the reason why we motivate the theory of generalized measurements in this chapter. It is clear, in most instances, that standard quantum measurement theory falls short in giving an accurate description of the measurement process. Nevertheless, there are certain circumstances where it holds perfectly. Interestingly, under certain conditions, we can extract projections from generalized observables. This we shall show later, in this chapter. A more in depth discussion of the shortcomings of the projection postulate can be found in [4, 59], however, we shall mention a few examples that we find very helpful to aid us to understand the quantum measurement process.

The first example is on the joint measurement of momentum and position of a quantum system. As pointed out by Wiseman and Milburn [59], the joint observation of a system’s position and momentum is completely acceptable for as long as we do not violate Heisenberg’s uncertainty principle [25]. However, If we assume that every measurement takes the form of a projection, then we can only measure one of the two observables, and not both, always. The second curious case involves the detection of photons. It is well known that detection of photons leads to their destruction, so detecting the number of photons, say in a cavity, leaves the system in a vacuum state and not the number eigenstate as dictated by the projection postulate.

We approach the theory of generalized measurement from the mathematical theory of measures. Indeed, generalized observables are described mathematically by positive operator-valued measures (POVM's) [57, 44]. Our method is to discuss measure theory starting from the basics, and hence this chapter contains mostly a collection of definitions and theorems, which we collected from [45, 2, 26].

2.2 Sample spaces and events

Definition 2.2.1. The set of all possible outcomes of a random experiment is called the *sample space*, denoted by Ω .

Definition 2.2.2. A subset of the sample space Ω , $A \subseteq \Omega$, is called an *event* and $\omega \in \Omega$ is called an *elementary event*.

2.3 Sigma algebra

Definition 2.3.1. Let Ω be a nonempty set and $\mathcal{P}(\Omega) \equiv \{A : A \subset \Omega\}$ be the power set of Ω . A collection of sets $\mathcal{F} \subset \mathcal{P}(\Omega)$ is called a *sigma algebra* if :

- a) $\Omega \in \mathcal{F}$,
- b) $A \in \mathcal{F} \Rightarrow A^c \in \mathcal{F}$, where set A^c is the complement of set A ,
- c) $A, B \in \mathcal{F} \Rightarrow A \cup B \in \mathcal{F}$,
- d) $A_n \in \mathcal{F}$, for $n \geq 1 \Rightarrow \bigcup_{n \geq 1} A_n \in \mathcal{F}$.

Note: A sigma algebra is always a monotone class, that is, \mathcal{F} contains a union of a sequence (A_n) for $n = 1, 2, \dots$ such that $A_n \in \mathcal{F}$ for each n , and $A_1 \subset A_2 \subset \dots$. It is also important to note that the smallest sigma algebra containing any non-empty family S of subsets A of Ω is identical with the smallest monotone class containing S . Given S and Ω the smallest sigma algebra containing S is the intersection of all sigma algebras containing S and the largest is the power set of Ω .

2.4 Measures, measurable space and measure space

Definition 2.4.1. Let Ω be a nonempty set and \mathcal{F} be a sigma algebra on Ω . Then, a set function μ on \mathcal{F} is called a *measure* if:

- a) $\mu(A) \geq 0$ for all $A \in \mathcal{F}$,

b) $\mu(\emptyset) = 0$,

c) for any disjoint collection of sets $A_1, A_2, \dots \in \mathcal{F}$ with $\bigcup_{n \geq 1} A_n \in \mathcal{F}$, $\mu(\bigcup_{n \geq 1} A_n) = \sum_{n=1}^{\infty} \mu(A_n)$.

Definition 2.4.2. The pair (Ω, \mathcal{F}) is called a *measurable space* and the triplet $(\Omega, \mathcal{F}, \mu)$ is called a *measure space*.

2.5 Probability measure and probability space

Definition 2.5.1. Let Ω be a nonempty set and \mathcal{F} be an algebra on Ω . Then, a set function p on \mathcal{F} is called a *probability measure* if it is a measure with the following extra properties:

a) $p(\Omega) = 1$,

b) $p(A^c) = 1 - p(A)$.

Definition 2.5.2. The triplet (Ω, \mathcal{F}, p) is called a *probability space*.

2.6 Random variables

Definition 2.6.1. A *random variable* is a function X that maps the elementary events ω of a probability space (Ω, \mathcal{F}, p) to an image space $X(\omega)$ which consists of real numbers.

Example 2.6.1. We look at an experiment in which we toss a coin. We define our random variable as

$$X = \begin{cases} 0 & \text{if heads,} \\ 1 & \text{if tails.} \end{cases}$$

The probability mass function is given by

$$p_X = \begin{cases} \frac{1}{2} & \text{if } X = 0, \\ \frac{1}{2} & \text{if } X = 1, \\ 0 & \text{otherwise.} \end{cases}$$

2.7 Joint and conditional probabilities

Definition 2.7.1. $p(A \cap B)$ is the *joint probability* that an event ω is contained in both sets A and B .

Definition 2.7.2. $p(A|B)$ is the *conditional probability* that events defined in set A occur in set B .

We define conditional probabilities in terms of joint probabilities as follows:

$$p(A|B) = p(A \cap B)/p(B),$$

also,

$$p(B|A) = p(A \cap B)/p(A).$$

Example 2.7.1. We propose an experiment in which a player has to pick a card from a standard 52-card deck. We want to determine the probability that a player picks a ‘picture card of hearts’. There are two ways we can do that. The first one is in which we sample from the full deck of cards. We count the number of ‘picture cards’ that have hearts on them. We find that there are 3 such cards. The probability is then given by dividing 3 by 52, the total number of cards in the deck, that is, $p = \frac{3}{52}$. Another way to determine the probability is to sample from a sub-deck containing ‘cards of hearts’ only which constitute a quarter of the full deck and apply the definition above. We define A , the set of events that the player picks a card of hearts, and B , the set of events that the player picks a picture card. We know that the probability $p(A)$ that the player picks a card of hearts is $\frac{1}{4}$, and the probability that a player picks a picture card if given a suit of hearts is $p(B|A) = \frac{3}{13}$. The joint probability that a player picks a picture card of hearts $p = p(B|A)p(A) = \frac{3}{13} \times \frac{1}{4} = \frac{3}{52}$.

2.8 Probability mass function and probability density

Definition 2.8.1. The *probability mass function* p_X is a function that gives the probabilities that a discrete random variable X takes certain values.

For continuous random variables we cannot use the probability mass function as the probability measure but the probability density function.

Definition 2.8.2. If $A(\omega', d\omega')$ is the set $\{\omega : \omega' \leq \omega < \omega' + d\omega'\}$, where ω are elementary events, then a function $\varrho(\omega')$ is a *probability density function* if $\varrho(\omega')d\omega' = p[A(\omega', d\omega')] \equiv p(\omega', d\omega')$. Normalization is given by $\int_{\Omega} \varrho(\omega')d\omega' = 1$.

2.9 Spectral measures and normal operators

Definition 2.9.1. A function P on the space (Ω, \mathcal{F}) whose domain is \mathcal{F} and values are self-adjoint projections in the Hilbert space \mathcal{H} is called a *spectral measure* on (Ω, \mathcal{F}) if it has the following properties:

- a) $P(\Omega) = \mathbb{1}$,
- b) $P(\emptyset) = 0$,
- c) $P(\bigcup_1^\infty A_j) = \sum_1^\infty P(A_j)$ for any sequence (A_j) of pairwise disjoint sets in \mathcal{F} ,
- d) If $A, B \in \mathcal{F}$ are disjoint then $P(A)P(B) = 0$,
- e) If $A \subset B \in \mathcal{F}$, then $P(A)P(B) = P(B)P(A) = P(A)$,
- f) For all $A, B \in \mathcal{F}$, we have $P(A \cap B) = P(A)P(B)$.

We are interested in the spectral representation of self-adjoint operators which we will apply later in the derivation of the master equations of continuous position measurement and estimation. At this point we appeal to the spectral theorem of self-adjoint operators.

Theorem 2.9.1. Let \hat{A} be a bounded self-adjoint (Hermitian) operator in the Hilbert space \mathcal{H} , there is a unique measure \hat{P} on the line supported in the interval $(-|a|, |a|)$, such that

$$\hat{A} = \int_{-|a|}^{|a|} x d\hat{P}(x), \quad (2.1)$$

where x is a eigenvalue of the operator \hat{A} . The function $\hat{P} : \mathcal{F} \rightarrow \mathcal{L}_P^+(\mathcal{H})$, where \mathcal{F} is a sigma algebra of the sample space and $\mathcal{L}_P^+(\mathcal{H})$ is the space of projection operators on the Hilbert space, is called a *projection-valued measure* (PVM).

2.10 Positive operator-valued measures (POVM)

Let Ω be the set of all possible measurement results i , \mathcal{F} be a sigma algebra over Ω and $|\psi\rangle \in \mathcal{H}$ be normalized, and the initial state of a quantum system. For each $i \in \Omega$ there exist a measurement operator (Kraus operator [34]) \hat{M}_i such that the probability $p(i)$ of obtaining the result i is given by Born's rule [8],

$$p(i) = \langle \psi | \hat{M}_i^\dagger \hat{M}_i | \psi \rangle, \quad (2.2)$$

and every time a measurement result i is obtained, the state of the system transforms as follows:

$$|\psi\rangle \xrightarrow{"i"} \frac{\hat{M}_i |\psi\rangle}{\sqrt{\langle \psi | \hat{M}_i^\dagger \hat{M}_i | \psi \rangle}}. \quad (2.3)$$

It is clear that the quantity on the right hand side of equation (2.2) is positive since it is the inner product of the state $|\psi'\rangle = \hat{M}_i|\psi\rangle$ with itself. Equation (2.2) also require that the following condition be satisfied:

$$\sum_i \hat{M}_i^\dagger \hat{M}_i = \mathbb{1}, \quad (2.4)$$

where $\mathbb{1}$ is the identity operator on our Hilbert space \mathcal{H} . Condition (2.4) is easy to prove using the measure theory we introduced above. We know that probability is a measure with the following property $p(\Omega) = 1$ and also $\Omega = \bigcup \{i\}$, the union of all $\{i\} \subset \Omega$, implying that $1 = p(\Omega) = p(\bigcup \{i\}) = \sum_i p(i) = \sum_i \langle \psi | \hat{M}_i^\dagger \hat{M}_i | \psi \rangle = \langle \psi | \left(\sum_i \hat{M}_i^\dagger \hat{M}_i \right) | \psi \rangle$. We also know that $1 = \langle \psi | \psi \rangle = \langle \psi | \mathbb{1} | \psi \rangle$. Comparing the last two expressions, we see that $\sum_i \hat{M}_i^\dagger \hat{M}_i = \mathbb{1}$. We can now define

a new set of positive operators $\hat{E}_i = \hat{M}_i^\dagger \hat{M}_i$ for each $i \in \Omega$ called *effects* of the measurements \hat{M}_i . The complete set of the effects \hat{E}_i form a positive operator valued measure $\hat{E} : \mathcal{F} \rightarrow \mathcal{L}^+(\mathcal{H})$, where \mathcal{F} is a sigma algebra of the sample space and $\mathcal{L}^+(\mathcal{H})$ is the space of positive operators on the Hilbert space. This is easy to verify since $\hat{E}_\Omega = \mathbb{1}$, $\hat{E}_\emptyset = \mathbf{0}$ and for each pair of disjoint sets $A, B \in \mathcal{F}$, $\hat{E}_{A \cup B} = \hat{E}_A + \hat{E}_B$.

2.10.1 Realization of POVM's

Generalized measurements on a quantum system can be realized by interacting the system with a smaller system, *ancillary*, and then performing a projective measurement on the ancillary as shown in the schematic below.

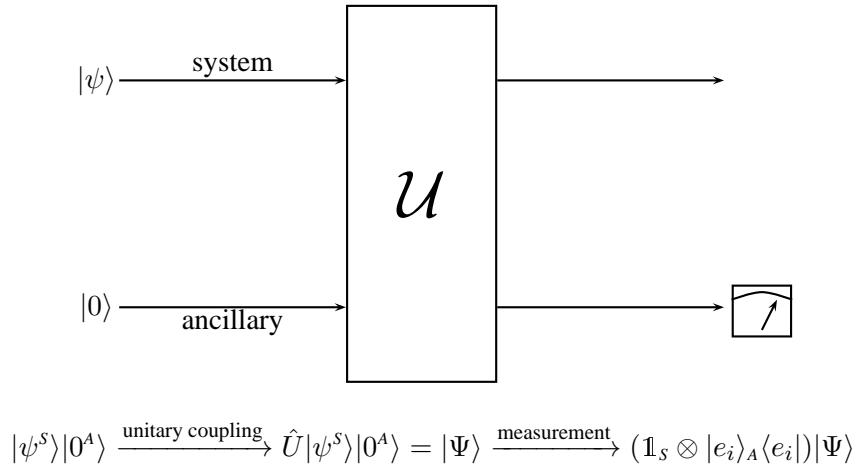


Figure 2.1: Schematic diagram showing the realization of generalized quantum measurement

In order for us to determine the state change of the system we must trace out the ancillary system's degrees of freedom from the state of the total system. We know that

$$\hat{\rho}(t)_{TOT} = |\Psi\rangle\langle\Psi| \xrightarrow{\text{measurement}} \hat{\rho}(t)'_{TOT} = \sum_i (\mathbb{1}_S \otimes |e_i\rangle_A \langle e_i|) |\Psi\rangle\langle\Psi| (\mathbb{1}_S \otimes |e_i\rangle_A \langle e_i|)^\dagger.$$

The change in the state of the system is therefore given by

$$\begin{aligned} \hat{\rho}(t)_S \rightarrow \hat{\rho}'_S(t) &= \text{tr}_A \{ \hat{\rho}(t)'_{TOT} \} = \text{tr}_A \left\{ \sum_i (\mathbb{1}_S \otimes |e_i\rangle_A \langle e_i|) U |\psi^S\rangle\langle 0^A| \langle \psi^S| \langle 0^A| U^\dagger (|e_i\rangle_A \langle e_i| \otimes \mathbb{1}_S) \right\} \\ &= \sum_{ij} \langle e_j^A | (\mathbb{1}_S \otimes |e_i\rangle_A \langle e_i|) U |\psi^S\rangle\langle 0^A| \langle \psi^S| \langle 0^A| U^\dagger (|e_i\rangle_A \langle e_i| \otimes \mathbb{1}_S) | e_j^A \rangle \\ &= \sum_{ij} \langle e_j^A | e_i^A \rangle \langle e_i^A | \hat{U} | 0^A \rangle |\psi^S\rangle\langle \psi^S| \langle 0^A | \hat{U}^\dagger | e_i^A \rangle \langle e_i^A | e_j^A \rangle \\ &= \sum_{ij} \delta_{ij} \langle e_i^A | \hat{U} | 0^A \rangle |\psi^S\rangle\langle \psi^S| \langle 0^A | \hat{U}^\dagger | e_i^A \rangle \delta_{ij} \\ &= \sum_i \langle e_i^A | \hat{U} | 0^A \rangle |\psi^S\rangle\langle \psi^S| \langle 0^A | \hat{U}^\dagger | e_i^A \rangle \\ &= \sum_i \langle e_i^A | \hat{U} | 0^A \rangle \hat{\rho}_S(t) \langle 0^A | \hat{U}^\dagger | e_i^A \rangle. \end{aligned} \tag{2.5}$$

It turns that the operation is a POVM on the state of the system with measurement operators $\hat{M}_i = \langle e_i^A | \hat{U} | 0^A \rangle$ and effects $\hat{E}_i = \langle 0^A | \hat{U}^\dagger | e_i^A \rangle \langle e_i^A | \hat{U} | 0^A \rangle = \langle 0^A | \hat{U}^\dagger \hat{P}_i^A \hat{U} | 0^A \rangle$, where $\hat{P}_i^A = |e_i^A\rangle\langle e_i^A|$ is a projector on the subspace of the ancillary system. We verify that the complete set of the effects constitute a POVM as follows:

$$\begin{aligned} \hat{E}_\Omega &= \sum_i \hat{M}_i^\dagger \hat{M}_i = \sum_i \langle 0^A | \hat{U}^\dagger \hat{P}_i^A \hat{U} | 0^A \rangle \\ &= \langle 0^A | \hat{U}^\dagger \left(\sum_i \hat{P}_i^A \right) \hat{U} | 0^A \rangle \\ &= \langle 0^A | \hat{U}^\dagger \mathbb{1}_A \hat{U} | 0^A \rangle \\ &= \langle 0^A | \hat{U}^\dagger \hat{U} | 0^A \rangle \\ &= \langle 0^A | \mathbb{1}_{TOT} | 0^A \rangle \\ &= \mathbb{1}_S, \end{aligned} \tag{2.6}$$

and for events $A', B' \in \mathcal{F}$ corresponding to measurement outcomes 1 and 2, and projections \hat{P}_1^A

and \hat{P}_2^A , respectively, on the ancillary system we have

$$\begin{aligned}
\hat{E}_{A' \cup B'} &= \langle 0^A | \hat{U}^\dagger \hat{P}_{A' \cup B'} \hat{U} | 0^A \rangle \\
&= \langle 0^A | \hat{U}^\dagger (\hat{P}_1^A + \hat{P}_2^A) \hat{U} | 0^A \rangle \\
&= \langle 0^A | \hat{U}^\dagger \hat{P}_1^A \hat{U} | 0^A \rangle + \langle 0^A | \hat{U}^\dagger \hat{P}_2^A \hat{U} | 0^A \rangle \\
&= \hat{E}_{A'} + \hat{E}_{B'}.
\end{aligned} \tag{2.7}$$

From equation (2.5) we can deduce that a POVM on a system can be seen as a projection on the system in a higher dimension and this is called *Naimark's dilation theorem* [42, 43, 29, 1, 37, 13].

Chapter 3

Continuous Measurement of Position

3.1 Introduction

The theory of continuous observation of quantum systems has been around for several decades. In 1987, Caves and Milburn [11] suggested a model for continuous measurement of position of a quantum system. This model is based on the theory of continuous quantum measurement as suggested, in 1982, by Barchielli [5] et al. In 1988, Diósi [14] then showed that continuous measurement of position in the selective regime can be represented by a certain Itô stochastic master equation. In this chapter we present a simplified approach to re-derive the master equations for continuous position measurement in both the selective and non-selective regimes, as well as the corresponding stochastic Schrödinger equations [55]. In this approach, we view continuous measurement as a sequence of unsharp measurements (see Figure 3.1) on a quantum system in the following limit:

$$\lim_{\substack{\tau \rightarrow 0 \\ \sigma \rightarrow \infty}} \frac{1}{\sigma^2 \tau} = \gamma, \quad (3.1)$$

where τ is the time interval between two consecutive measurements, σ is the precision parameter of measurement and γ is a finite quantity called the decoherence rate. For historical reasons we refer to this limit as the Barchielli limit, because Barchielli and his co-authors were the first people to use this type of limit.

Unsharp measurement is achieved by selecting generalized measurement observables, which are commuting positive operator valued measures (POVM), rather than the standard von Neumann projection operators, which are projection valued measures (PVM). We consider a special kind of unsharp measurement of position in one spatial dimension x given by the following Kraus operators [34]:

$$\hat{M}_{\bar{x}} = \frac{1}{\sqrt[4]{2\pi\sigma^2}} \exp\left(-\frac{(\hat{x} - \bar{x})^2}{4\sigma^2}\right), \quad (3.2)$$

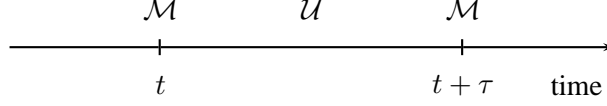


Figure 3.1: Schematic diagram for the time evolution of a system undergoing a sequence of measurements \hat{M} at time intervals τ . Between two consecutive measurements the closed system evolves unitarily.

where \bar{x} are measurement results. The effects of the measurements are Gaussian and given by:

$$\hat{M}_{\bar{x}}^\dagger \hat{M}_{\bar{x}} = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(\hat{x} - \bar{x})^2}{2\sigma^2}\right). \quad (3.3)$$

These operators satisfy two necessary conditions. The first one is the completeness condition:

$$\begin{aligned} \int_{-\infty}^{\infty} d\bar{x} \hat{M}_{\bar{x}}^\dagger \hat{M}_{\bar{x}} &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{(\hat{x} - \bar{x})^2}{2\sigma^2}\right) d\bar{x} \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{(x - \bar{x})^2}{2\sigma^2}\right) d\bar{x} \int_{-\infty}^{\infty} |x\rangle\langle x| dx = \mathbb{1}. \end{aligned} \quad (3.4)$$

The second is the ability to extract a projection in the limit $\sigma \rightarrow 0$ as shown below:

$$\begin{aligned} \lim_{\sigma \rightarrow 0} \hat{M}_{\bar{x}}^\dagger \hat{M}_{\bar{x}} &= \lim_{\sigma \rightarrow 0} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(\hat{x} - \bar{x})^2}{2\sigma^2}\right) \\ &= \lim_{\sigma \rightarrow 0} \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x - \bar{x})^2}{2\sigma^2}\right) |x\rangle\langle x| dx \\ &= \int_{-\infty}^{\infty} \delta(x - \bar{x}) |x\rangle\langle x| dx \\ &= |\bar{x}\rangle\langle \bar{x}|, \end{aligned} \quad (3.5)$$

where δ is the Dirac delta function [16]. The unitary evolution between two consecutive measurements is given by

$$\hat{U} = \exp\left(-\frac{i}{\hbar} \hat{H} \tau\right). \quad (3.6)$$

In order for us to derive the state evolution equations it is necessary to Taylor-expand both the measurement operator $\hat{M}_{\bar{x}}$ and unitary operator \hat{U} . We expand the unitary operator up to the first order with respect to the time interval τ as follows:

$$\hat{U} = \mathbb{1} - \frac{i}{\hbar} \hat{H} \tau + \mathcal{O}(\tau^2), \quad (3.7)$$

because higher order terms in τ vanish in the Barchielli limit. We expand the measurement operators with respect to $\frac{\bar{x}}{\sigma^2}$ and derive the third line of the following:

$$\begin{aligned} \hat{M}_{\bar{x}} &= \frac{1}{\sqrt{4\pi\sigma^2}} \exp\left(-\frac{(\hat{x} - \bar{x})^2}{4\sigma^2}\right) \\ &= \frac{1}{\sqrt{4\pi\sigma^2}} \exp\left(-\frac{\bar{x}^2}{4\sigma^2}\right) \exp\left(\frac{-\hat{x}^2 + 2\hat{x}\bar{x}}{4\sigma^2}\right) \\ &= \frac{1}{\sqrt{4\pi\sigma^2}} \exp\left(-\frac{\bar{x}^2}{4\sigma^2}\right) \left(1 - \frac{\hat{x}^3\bar{x}}{8\sigma^4} + \frac{\hat{x}^2\bar{x}^2}{8\sigma^4} + \frac{\hat{x}\bar{x}}{2\sigma^2} + \frac{\hat{x}^4}{32\sigma^4} - \frac{\hat{x}^2}{4\sigma^2} + \mathcal{O}(\sigma^{-6})\right). \end{aligned} \quad (3.8)$$

We truncated the expansion above as follows: while all other terms in σ of order ≤ -4 vanish in the Barchielli limit, the terms in $\frac{\bar{x}^2}{\sigma^4}$ survive.

3.2 Derivation of the master equation for measurement of position in the non-selective regime

Consider an experiment in which we perform unsharp position measurements in a sequence as shown in figure 3.1. If the state of the system at a time t is represented by the density operator $\hat{\rho}(t)$ then after a time τ the state of the system

$$\begin{aligned} \hat{\rho}(t) &\rightarrow \hat{\rho}(t + \tau) = \int_{-\infty}^{\infty} d\bar{x} \hat{U} \hat{M}_{\bar{x}} \hat{\rho}(t) \hat{M}_{\bar{x}}^\dagger \hat{U}^\dagger \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \hat{U} \left(\int_{-\infty}^{\infty} d\bar{x} \exp\left(\frac{-(\hat{x} - \bar{x})^2}{4\sigma^2}\right) \hat{\rho}(t) \exp\left(\frac{-(\hat{x} - \bar{x})^2}{4\sigma^2}\right) \right) \hat{U}^\dagger. \end{aligned} \quad (3.9)$$

To solve the integral in equation (3.9) we need apply some commutative super-algebra which was introduced in [3, 32]. We define new position operators \hat{x}_L and \hat{x}_R as follows:

$$\hat{x}_L \hat{\rho}(t) \equiv \hat{\rho}(t) \hat{x}_L := \hat{x} \hat{\rho}(t) \quad (3.10)$$

and

$$\hat{x}_R \hat{\rho}(t) \equiv \hat{\rho}(t) \hat{x}_R := \hat{\rho}(t) \hat{x}. \quad (3.11)$$

Assuming that the operator \hat{x} has the following spectral representation:

$$\hat{x} = \int_{-\infty}^{\infty} x d\hat{P}(x), \quad (3.12)$$

where x are position eigenvalues, $d\hat{P}(x) = |x\rangle\langle x|dx$ and $\hat{P}(x)$ are a family of commuting orthogonal projectors with the following properties [10]:

$$\hat{P}(x') \geq \hat{P}(x) \text{ for } x' > x, \quad (3.13)$$

$$\lim_{\epsilon \rightarrow +0} \hat{P}(x + \epsilon) = \hat{P}(x), \quad (3.14)$$

$$\lim_{x \rightarrow -\infty} \hat{P}(x) = 0 \quad (3.15)$$

and

$$\lim_{x \rightarrow +\infty} \hat{P}(x) = \mathbb{1}, \quad (3.16)$$

then the operators \hat{x}_L and \hat{x}_R can be written as follows:

$$\hat{x}_L = \int_{-\infty}^{\infty} x' d\hat{P}_L(x') \quad (3.17)$$

and

$$\hat{x}_R = \int_{-\infty}^{\infty} x'' d\hat{P}_R(x''). \quad (3.18)$$

The actions of the operators $d\hat{P}_L(x')$ and $d\hat{P}_R(x'')$ on any arbitrary operator \hat{A} of the system's Hilbert space \mathcal{H} are defined as follows:

$$d\hat{P}_L(x')\hat{A} \equiv \hat{A} d\hat{P}_L(x') := d\hat{P}(x) \hat{A} \quad (3.19)$$

and

$$d\hat{P}_R(x'')\hat{A} \equiv \hat{A} d\hat{P}_R(x'') := \hat{A} d\hat{P}(x), \quad (3.20)$$

respectively. The equations (3.19) and (3.20) are consistent with equations (3.10) and (3.11). The operators \hat{x}_L and \hat{x}_R commute with all operators of the Hilbert space and therefore we can rewrite equation (3.9) as follows:

$$\begin{aligned} \hat{\rho}(t + \tau) &= \frac{1}{\sqrt{2\pi\sigma^2}} \hat{U} \left(\int_{-\infty}^{\infty} d\bar{x} \exp \left(\frac{-(\hat{x}_L - \bar{x})^2 - (\hat{x}_R - \bar{x})^2}{4\sigma^2} \right) \right) \hat{\rho}(t) \hat{U}^\dagger \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \hat{U} \left(\int_{-\infty}^{\infty} d\bar{x} \exp \left(-\frac{1}{2\sigma^2} \bar{x}^2 + \frac{\hat{x}_L + \hat{x}_R}{2\sigma^2} \bar{x} - \frac{\hat{x}_L^2 + \hat{x}_R^2}{4\sigma^2} \right) \right) \hat{\rho}(t) \hat{U}^\dagger. \end{aligned} \quad (3.21)$$

We now apply equations (3.17) and (3.18) to the integral in equation (3.21) as follows:

$$\begin{aligned}
& \int_{-\infty}^{\infty} d\bar{x} \exp \left(-\frac{1}{2\sigma^2} \bar{x}^2 + \frac{\hat{x}_L + \hat{x}_R}{2\sigma^2} \bar{x} - \frac{\hat{x}_L^2 + \hat{x}_R^2}{4\sigma^2} \right) \\
&= \int_{-\infty}^{\infty} d\bar{x} \exp \left(-\frac{1}{2\sigma^2} \bar{x}^2 \right) \times \exp \left(\frac{\hat{x}_L}{2\sigma^2} \bar{x} - \frac{\hat{x}_L^2}{4\sigma^2} \right) \times \exp \left(\frac{\hat{x}_R}{2\sigma^2} \bar{x} - \frac{\hat{x}_R^2}{4\sigma^2} \right) \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} d\bar{x} \exp \left(-\frac{1}{2\sigma^2} \bar{x}^2 \right) \right. \\
&\quad \times \exp \left(\frac{x'}{2\sigma^2} \bar{x} - \frac{(x')^2}{4\sigma^2} \right) \times \exp \left(\frac{x''}{2\sigma^2} \bar{x} - \frac{(x'')^2}{4\sigma^2} \right) \Big] d\hat{P}_L(x') d\hat{P}_R(x'') \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} d\bar{x} \exp \left(-\frac{1}{2\sigma^2} \bar{x}^2 + \frac{x' + x''}{2\sigma^2} \bar{x} - \frac{(x')^2 + (x'')^2}{4\sigma^2} \right) \right] d\hat{P}_L(x') d\hat{P}_R(x''). \quad (3.22)
\end{aligned}$$

We can now evaluate the square bracketed integral in equation (3.22) using standard procedure because the exponential does not contain operators, but rather numbers. We evaluate the integral as follows:

$$\begin{aligned}
& \int_{-\infty}^{\infty} d\bar{x} \exp \left(-\frac{1}{2\sigma^2} \bar{x}^2 + \frac{x' + x''}{2\sigma^2} \bar{x} - \frac{(x')^2 + (x'')^2}{4\sigma^2} \right) \\
&= \sqrt{2\pi\sigma^2} \exp \left(-\frac{1}{8\sigma^2} ((x')^2 + (x'')^2 - 2x'x'') \right) \\
&= \sqrt{2\pi\sigma^2} \left(1 - \frac{1}{8\sigma^2} ((x')^2 + (x'')^2 - 2x'x'') + \mathcal{O}(\sigma^{-4}) \right). \quad (3.23)
\end{aligned}$$

Substituting equation (3.23) into equation (3.22) yields the following:

$$\begin{aligned}
& \int_{-\infty}^{\infty} d\bar{x} \exp \left(-\frac{1}{2\sigma^2} \bar{x}^2 + \frac{\hat{x}_L + \hat{x}_R}{2\sigma^2} \bar{x} - \frac{\hat{x}_L^2 + \hat{x}_R^2}{4\sigma^2} \right) \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\sqrt{2\pi\sigma^2} \left(1 - \frac{1}{8\sigma^2} ((x')^2 + (x'')^2 - 2x'x'') + \mathcal{O}(\sigma^{-4}) \right) \right] d\hat{P}_L(x') d\hat{P}_R(x'') \\
&= \sqrt{2\pi\sigma^2} \left(\mathbb{1} - \frac{1}{8\sigma^2} (\hat{x}_L^2 + \hat{x}_R^2 - 2\hat{x}_L\hat{x}_R) + \mathcal{O}(\sigma^{-4}) \right). \quad (3.24)
\end{aligned}$$

We now substitute equations (3.7) and (3.24) into equation (3.21) to obtain the following equation:

$$\begin{aligned}
\hat{\rho}(t + \tau) &= (\mathbb{1} - \frac{i}{\hbar} \hat{H} \tau + \mathcal{O}(\tau^2)) (\mathbb{1} - \frac{1}{8\sigma^2} (\hat{x}_L^2 + \hat{x}_R^2 - 2\hat{x}_L \hat{x}_R) + \mathcal{O}(\sigma^{-4})) \hat{\rho}(t) \\
&\times (\mathbb{1} + \frac{i}{\hbar} \hat{H} \tau + \mathcal{O}(\tau^2)) \\
&= (\mathbb{1} - \frac{i}{\hbar} \hat{H} \tau + \mathcal{O}(\tau^2)) (\hat{\rho}(t) - \frac{1}{8\sigma^2} \hat{x}^2 \hat{\rho}(t) + \hat{\rho}(t) \hat{x}^2 - 2\hat{x} \hat{\rho}(t) \hat{x} + \mathcal{O}(\sigma^{-4})) \\
&\times (\mathbb{1} + \frac{i}{\hbar} \hat{H} \tau + \mathcal{O}(\tau^2)) \\
&= (\mathbb{1} - \frac{i}{\hbar} \hat{H} \tau + \mathcal{O}(\tau^2)) (\hat{\rho}(t) - \frac{1}{8\sigma^2} [\hat{x}, [\hat{x}, \hat{\rho}(t)]] + \mathcal{O}(\sigma^{-4})) (\mathbb{1} + \frac{i}{\hbar} \hat{H} \tau + \mathcal{O}(\tau^2)) \\
&= \hat{\rho}(t) - \frac{i}{\hbar} [\hat{H}, \hat{\rho}(t)] \tau - \frac{1}{8\sigma^2} [\hat{x}, [\hat{x}, \hat{\rho}(t)]] + \frac{i\tau}{8\hbar\sigma^2} [\hat{H}, [\hat{x}, [\hat{x}, \hat{\rho}(t)]]] + \mathcal{O}(\tau^2) + \mathcal{O}(\sigma^{-4}). \quad (3.25)
\end{aligned}$$

We can infer from equation (3.25) that,

$$\begin{aligned}
\Delta \hat{\rho}(t) &= \hat{\rho}(t + \tau) - \hat{\rho}(t) \\
&= -\frac{i}{\hbar} [\hat{H}, \hat{\rho}(t)] \tau - \frac{1}{8\sigma^2} [\hat{x}, [\hat{x}, \hat{\rho}(t)]] \tau + \frac{i\tau}{8\hbar\sigma^2} [\hat{H}, [\hat{x}, [\hat{x}, \hat{\rho}(t)]]] + \mathcal{O}(\tau^2) + \mathcal{O}(\sigma^{-4}). \quad (3.26)
\end{aligned}$$

Applying the Barchielli limit to equation (3.26) yields the following:

$$d\hat{\rho}(t) = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}(t)] dt - \frac{\gamma}{8} [\hat{x}, [\hat{x}, \hat{\rho}(t)]] dt. \quad (3.27)$$

We note that the higher order terms in τ vanish as τ approaches 0. Equation (3.27) is the master equation of continuous position measurement in the non-selective regime.

3.3 Derivation of the stochastic master equation

The stochastic master equation for the continuous measurement of position of a quantum system in the selective regime was given by Diósi [14]. In this section we present an alternative way to derive this master equation. As in the previous section we consider the same experiment but the only difference now is that we account for the measurement results. We start our derivation the same way as we did in the previous section, with the state of the system at a time t being represented by the density operator $\hat{\rho}(t)$. After a time τ the state of the system reads

$$\hat{\rho}(t + \tau) = \frac{1}{p_{\hat{\rho}}(\bar{x})} \hat{U} \hat{M}_{\bar{x}} \hat{\rho}(t) \hat{M}_{\bar{x}}^\dagger \hat{U}^\dagger, \quad (3.28)$$

where $p_{\hat{\rho}}(\bar{x})$ is the probability of obtaining the measurement result \bar{x} and is given by:

$$\begin{aligned}
p_{\hat{\rho}}(\bar{x}) &= \text{tr} \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{(\hat{x} - \bar{x})^2}{2\sigma^2} \right) \hat{\rho}(t) \right\} \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \text{tr} \left\{ \exp \left(-\frac{\hat{x}^2 - 2\bar{x}\hat{x} + \bar{x}^2}{2\sigma^2} \right) \hat{\rho}(t) \right\} \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{\bar{x}^2}{2\sigma^2} \right) \text{tr} \left\{ \exp \left(-\frac{\hat{x}^2 - 2\bar{x}\hat{x}}{2\sigma^2} \right) \hat{\rho}(t) \right\} \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{\bar{x}^2}{2\sigma^2} \right) \text{tr} \left\{ \left(\mathbb{1} - \frac{\hat{x}^2 - 2\bar{x}\hat{x}}{2\sigma^2} + \frac{1}{2!} \left(-\frac{\hat{x}^2 - 2\bar{x}\hat{x}}{2\sigma^2} \right)^2 + \mathcal{O}(\sigma^{-6}) \right) \hat{\rho}(t) \right\} \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{\bar{x}^2}{2\sigma^2} \right) \text{tr} \left\{ \left(\mathbb{1} + \frac{\bar{x}}{\sigma^2} \hat{x} - \overbrace{\left(\frac{1}{2\sigma^2} - \frac{\bar{x}^2}{2\sigma^4} \right)}^{=0 \text{ in the limit}} \hat{x}^2 \right. \right. \\
&\quad \left. \left. - \frac{\bar{x}}{2\sigma^4} \hat{x}^3 + \frac{1}{8\sigma^4} \hat{x}^4 + \mathcal{O}(\sigma^{-6}) \right) \hat{\rho}(t) \right\} \\
&\quad \text{vanish in the limit} \\
&\approx \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{\bar{x}^2}{2\sigma^2} \right) \left(\text{tr} \left\{ \hat{\rho}(t) \right\} + \text{tr} \left\{ \frac{\bar{x}\hat{x}}{\sigma^2} \hat{\rho}(t) \right\} \right) \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{\bar{x}^2}{2\sigma^2} \right) \left(1 + \frac{\bar{x}}{\sigma^2} \langle \hat{x} \rangle_{\hat{\rho}} \right). \tag{3.29}
\end{aligned}$$

The quantity $\frac{1}{p_{\hat{\rho}}(\bar{x})}$ in equation (3.28) can conveniently be Taylor-expanded as follows:

$$\frac{1}{p_{\hat{\rho}}(\bar{x})} \approx \sqrt{2\pi\sigma^2} \exp \left(\frac{\bar{x}^2}{2\sigma^2} \right) \left(1 - \frac{\bar{x}}{\sigma^2} \langle \hat{x} \rangle_{\hat{\rho}} + \frac{\bar{x}^2}{\sigma^4} \langle \hat{x} \rangle_{\hat{\rho}}^2 \right). \tag{3.30}$$

To simplify the evaluation of equation (3.28) we first simplify the measurement part,

$$\frac{1}{p_{\hat{\rho}}(\bar{x})} \hat{M}_{\bar{x}} \hat{\rho}(t) \hat{M}_{\bar{x}}^{\dagger}, \tag{3.31}$$

by substituting equations (3.30) and (3.8) as follows:

$$\begin{aligned}
& \frac{\hat{M}_{\bar{x}}\hat{\rho}(t)\hat{M}_{\bar{x}}^\dagger}{p_{\hat{\rho}}(\bar{x})} \\
&= \left(1 - \frac{\bar{x}}{\sigma^2}\langle\hat{x}\rangle_{\hat{\rho}} + \frac{\bar{x}^2}{\sigma^4}\langle\hat{x}\rangle_{\hat{\rho}}^2\right) \left(\mathbb{1} - \frac{\hat{x}^3\bar{x}}{8\sigma^4} + \frac{\hat{x}^2\bar{x}^2}{8\sigma^4} + \frac{\hat{x}\bar{x}}{2\sigma^2} + \frac{\hat{x}^4}{32\sigma^4} - \frac{\hat{x}^2}{4\sigma^2} + \mathcal{O}(\sigma^{-6})\right) \hat{\rho}(t) \\
&\quad \times \left(\mathbb{1} - \frac{\hat{x}^3\bar{x}}{8\sigma^4} + \frac{\hat{x}^2\bar{x}^2}{8\sigma^4} + \frac{\hat{x}\bar{x}}{2\sigma^2} + \frac{\hat{x}^4}{32\sigma^4} - \frac{\hat{x}^2}{4\sigma^2} + \mathcal{O}(\sigma^{-6})\right) \\
&= \left(1 - \frac{\bar{x}}{\sigma^2}\langle\hat{x}\rangle_{\hat{\rho}} + \frac{\bar{x}^2}{\sigma^4}\langle\hat{x}\rangle_{\hat{\rho}}^2\right) \left(\hat{\rho}(t) + \frac{\bar{x}}{2\sigma^2}\hat{x}\hat{\rho}(t) + \frac{\bar{x}}{2\sigma^2}\hat{\rho}(t)\hat{x} - \frac{1}{4\sigma^2}\hat{x}^2\hat{\rho}(t) - \frac{1}{4\sigma^2}\hat{\rho}(t)\hat{x}^2\right. \\
&\quad + \frac{\bar{x}^2}{8\sigma^4}\hat{x}^2\hat{\rho}(t) + \frac{\bar{x}^2}{8\sigma^4}\hat{\rho}(t)\hat{x}^2 + \frac{\bar{x}^2}{4\sigma^4}\hat{x}\hat{\rho}(t)\hat{x} - \frac{\bar{x}}{8\sigma^4}\hat{x}^3\hat{\rho}(t) - \frac{\bar{x}}{8\sigma^4}\hat{\rho}(t)\hat{x}^3 \\
&\quad + \frac{1}{32\sigma^4}\hat{x}^4\hat{\rho}(t) + \frac{1}{32\sigma^4}\hat{\rho}(t)\hat{x}^4 - \frac{\bar{x}}{4\sigma^4}\hat{x}^2\hat{\rho}(t)\hat{x} + \frac{1}{16\sigma^4}\hat{x}^2\hat{\rho}(t)\hat{x}^2 + \mathcal{O}(\sigma^{-6})) \\
&= \left(1 - \frac{\bar{x}}{\sigma^2}\langle\hat{x}\rangle_{\hat{\rho}} + \frac{\bar{x}^2}{\sigma^4}\langle\hat{x}\rangle_{\hat{\rho}}^2\right) \left(\hat{\rho}(t) + \frac{\bar{x}}{2\sigma^2}\{\hat{x}, \hat{\rho}(t)\} - \frac{1}{8\sigma^2}[\hat{x}, [\hat{x}, \hat{\rho}(t)]] - \frac{1}{8\sigma^2}\{\hat{x}, \{\hat{x}, \hat{\rho}(t)\}\}\right. \\
&\quad + \frac{\bar{x}^2}{8\sigma^4}\{\hat{x}, \{\hat{x}, \hat{\rho}(t)\}\} - \frac{\bar{x}}{8\sigma^4}\{\hat{x}^3, \hat{\rho}(t)\} + \frac{1}{32\sigma^4}\{\hat{x}^4, \hat{\rho}(t)\} \\
&\quad \left. - \frac{\bar{x}}{4\sigma^4}\hat{x}^2\hat{\rho}(t)\hat{x} + \frac{1}{16\sigma^4}\hat{x}^2\hat{\rho}(t)\hat{x}^2 + \mathcal{O}(\sigma^{-6})\right). \tag{3.32}
\end{aligned}$$

After applying the Barchielli limit, equation (3.32) becomes:

$$\begin{aligned}
& \frac{\hat{M}_{\bar{x}}\hat{\rho}(t)\hat{M}_{\bar{x}}^\dagger}{p_{\hat{\rho}}(\bar{x})} \\
&= \left(1 - \bar{x}\tau\gamma\langle\hat{x}\rangle_{\hat{\rho}} + \bar{x}^2\tau^2\gamma^2\langle\hat{x}\rangle_{\hat{\rho}}^2\right) \left(\hat{\rho}(t) + \frac{\bar{x}\tau\gamma}{2}\{\hat{x}, \hat{\rho}(t)\} - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}(t)]]\right. \\
&\quad - \frac{\tau\gamma}{8}\{\hat{x}, \{\hat{x}, \hat{\rho}(t)\}\} + \frac{\bar{x}^2\tau^2\gamma^2}{8}\{\hat{x}, \{\hat{x}, \hat{\rho}(t)\}\} - \frac{\bar{x}\tau^2\gamma^2}{8}\{\hat{x}^3, \hat{\rho}(t)\} + \frac{\tau^2\gamma^2}{32}\{\hat{x}^4, \hat{\rho}(t)\} \\
&\quad \left. - \frac{\bar{x}\tau^2\gamma^2}{4}\hat{x}^2\hat{\rho}(t)\hat{x} + \frac{\tau^2\gamma^2}{16}\hat{x}^2\hat{\rho}(t)\hat{x}^2 + \mathcal{O}(\tau^3)\right). \tag{3.33}
\end{aligned}$$

In order for us to further simplify equation (3.33), we need to first introduce some stochastic calculus, which was suggested by Diósi [14, 15] where our measurement results \bar{x}_t at a time t are governed by the following *heuristic* stochastic equation:

$$\bar{x}_t = \langle\hat{x}\rangle_{\hat{\rho}(t)} + \frac{1}{\sqrt{\gamma}}w_t, \tag{3.34}$$

where w_t is standard white noise which is defined by

$$\langle w_t \rangle_{st} = 0 \tag{3.35}$$

and

$$\langle w_t w_s \rangle_{st} = \delta(t - s). \quad (3.36)$$

However, equation (3.34) is not time differentiable because w_t is not a real function of time. To work around this problem we introduce the quantity Q_t , which is the time integrated measurement signal and defined as follows:

$$Q_t := \int_0^t \bar{x}_{t'} dt'. \quad (3.37)$$

Now substituting for $\bar{x}_{t'}$ in equation (3.37),

$$\begin{aligned} Q_t &:= \int_0^t \left(\langle \hat{x} \rangle_{\hat{\rho}(t')} + \frac{1}{\sqrt{\gamma}} w_{t'} \right) dt' \\ &= \langle \hat{x} \rangle_{\hat{\rho}(t)} t + \frac{1}{\sqrt{\gamma}} W_t, \end{aligned} \quad (3.38)$$

where W_t , the time integral of w_t is a Wiener process. From equation (3.38) it follows that

$$dQ = \langle \hat{x} \rangle_{\hat{\rho}} dt + \gamma^{-\frac{1}{2}} dW, \quad (3.39)$$

where dW are Wiener increments and satisfy the following Itô rules:

$$\langle dW \rangle_{st} = 0, \quad (3.40)$$

$$(dW)^2 = dt, \quad (3.41)$$

$$(dW)^n = 0, \text{ for } n > 2. \quad (3.42)$$

We note that in the Barchielli limit $\bar{x}\tau \equiv dQ$ implying that $\bar{x}^2\tau^2 = (dQ)^2 = \frac{1}{\gamma}dt$. Substituting dQ for $\bar{x}\tau$ into equation (3.33) we obtain:

$$\begin{aligned} &\frac{\hat{M}_{\bar{x}} \hat{\rho}(t) \hat{M}_{\bar{x}}^\dagger}{p_{\hat{\rho}}(\bar{x})} \\ &= \left(1 - (dQ)\gamma \langle \hat{x} \rangle_{\hat{\rho}} + (dQ)^2 \gamma^2 \langle \hat{x}^2 \rangle_{\hat{\rho}} \right) \left(\hat{\rho}(t) + \frac{(dQ)\gamma}{2} \{ \hat{x}, \hat{\rho}(t) \} - \frac{\tau\gamma}{8} [\hat{x}, [\hat{x}, \hat{\rho}(t)]] \right) \\ &\quad - \frac{\tau\gamma}{8} \{ \hat{x}, \{ \hat{x}, \hat{\rho}(t) \} \} + \frac{(dQ)^2 \gamma^2}{8} \{ \hat{x}, \{ \hat{x}, \hat{\rho}(t) \} \} - \frac{(dQ)\tau\gamma^2}{8} \{ \hat{x}^3, \hat{\rho}(t) \} \\ &\quad + \frac{\tau^2 \gamma^2}{32} \{ \hat{x}^4, \hat{\rho}(t) \} - \frac{(dQ)\tau\gamma^2}{4} \hat{x}^2 \hat{\rho}(t) \hat{x} + \frac{\tau^2 \gamma^2}{16} \hat{x}^2 \hat{\rho}(t) \hat{x}^2 + \mathcal{O}(\sigma^{-6}). \end{aligned} \quad (3.43)$$

We now apply Itô rules to equation (3.43) to obtain the following:

$$\begin{aligned}
& \frac{\hat{M}_{\bar{x}}\hat{\rho}(t)\hat{M}_{\bar{x}}^\dagger}{p_{\hat{\rho}}(\bar{x})} \\
&= \left(1 - (dQ)\gamma\langle\hat{x}\rangle_{\hat{\rho}} + \tau\gamma\langle\hat{x}\rangle_{\hat{\rho}}^2\right) \left(\hat{\rho}(t) + \frac{(dQ)\gamma}{2}\{\hat{x}, \hat{\rho}(t)\} - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}(t)]]\right) \\
&\quad - \frac{\tau\gamma}{8}\{\hat{x}, \{\hat{x}, \hat{\rho}(t)\}\} + \frac{\tau\gamma^2}{8\gamma}\{\hat{x}, \{\hat{x}, \hat{\rho}(t)\}\} \\
&= \left(1 - (dQ)\gamma\langle\hat{x}\rangle_{\hat{\rho}} + \tau\gamma\langle\hat{x}\rangle_{\hat{\rho}}^2\right) \left(\hat{\rho}(t) + \frac{(dQ)\gamma}{2}\{\hat{x}, \hat{\rho}(t)\} - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}(t)]]\right) \\
&= \hat{\rho}(t) - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}(t)]] + \frac{(dQ)\gamma}{2}\{\hat{x}, \hat{\rho}(t)\} - (dQ)\gamma\hat{\rho}(t)\langle\hat{x}\rangle_{\hat{\rho}} \\
&\quad - \frac{\tau\gamma\langle\hat{x}\rangle_{\hat{\rho}}}{2}\{\hat{x}, \hat{\rho}(t)\} + \tau\gamma\langle\hat{x}\rangle_{\hat{\rho}}^2\hat{\rho}(t) \\
&= \hat{\rho}(t) - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}(t)]] + \frac{(dQ)\gamma}{2}\{\hat{x} - \langle\hat{x}\rangle_{\hat{\rho}}, \hat{\rho}(t)\} - \frac{\tau\gamma\langle\hat{x}\rangle_{\hat{\rho}}}{2}\{\hat{x} - \langle\hat{x}\rangle_{\hat{\rho}}, \hat{\rho}(t)\} \\
&= \hat{\rho}(t) - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}(t)]] + \frac{\gamma}{2}\{\hat{x} - \langle\hat{x}\rangle_{\hat{\rho}}, \hat{\rho}(t)\}(dQ - \tau\langle\hat{x}\rangle_{\hat{\rho}}). \tag{3.44}
\end{aligned}$$

Substituting equations (3.7) and (3.44) into (3.28), yields the following:

$$\begin{aligned}
& \hat{\rho}(t + \tau) \\
&= \frac{1}{p_{\hat{\rho}}(\bar{x})}\hat{U}\hat{M}_{\bar{x}}\hat{\rho}(t)\hat{M}_{\bar{x}}^\dagger\hat{U}^\dagger \\
&= \left(\mathbb{1} - \frac{i}{\hbar}\hat{H}\tau + \mathcal{O}(\tau^2)\right) \left(\hat{\rho}(t) - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}(t)]] + \frac{\gamma}{2}\{\hat{x} - \langle\hat{x}\rangle_{\hat{\rho}}, \hat{\rho}(t)\}(dQ - \tau\langle\hat{x}\rangle_{\hat{\rho}})\right) \\
&\quad \times \left(\mathbb{1} + \frac{i}{\hbar}\hat{H}\tau + \mathcal{O}(\tau^2)\right) \\
&= \hat{\rho}(t) - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}(t)]] + \frac{\gamma}{2}\{\hat{x} - \langle\hat{x}\rangle_{\hat{\rho}}, \hat{\rho}(t)\}(dQ - \tau\langle\hat{x}\rangle_{\hat{\rho}}) - \frac{i}{\hbar}\hat{H}\tau\hat{\rho}(t) + \hat{\rho}(t)\frac{i}{\hbar}\hat{H}\tau \\
&= \hat{\rho}(t) - \frac{i\tau}{\hbar}[\hat{H}, \hat{\rho}(t)] - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}(t)]] + \frac{\gamma}{2}\{\hat{x} - \langle\hat{x}\rangle_{\hat{\rho}}, \hat{\rho}(t)\}(dQ - \tau\langle\hat{x}\rangle_{\hat{\rho}}). \tag{3.45}
\end{aligned}$$

For infinitesimal increments of time τ , which we shall denote by the familiar dt , the change in the system density operator $\Delta\hat{\rho} = \hat{\rho}(t + \tau) - \hat{\rho}(t)$ becomes infinitesimal and hence we shall represent it by $d\hat{\rho}$. We can therefore write the following stochastic differential equation:

$$\begin{aligned}
d\hat{\rho}(t) &= -\frac{i}{\hbar}[\hat{H}, \hat{\rho}(t)]dt - \frac{\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}(t)]]dt + \frac{\gamma}{2}\{\hat{x} - \langle\hat{x}\rangle_{\hat{\rho}}, \hat{\rho}(t)\}(dQ - \langle\hat{x}\rangle_{\hat{\rho}}dt) \\
&= -\frac{i}{\hbar}[\hat{H}, \hat{\rho}(t)]dt - \frac{\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}(t)]]dt + \frac{\sqrt{\gamma}}{2}\{\hat{x} - \langle\hat{x}\rangle_{\hat{\rho}}, \hat{\rho}(t)\}dW, \tag{3.46}
\end{aligned}$$

as the master equation for continuous measurement of position in the selective regime.

3.4 Derivation of the Itô stochastic Schrödinger equation

Even though the master equation that we derived in the previous section can be used to evolve pure states, it is more convenient to evolve them by Schrödinger-type equations [23]. In this section we re-derive the stochastic Schrödinger equation that governs the evolution of the state vector or wave function of a quantum system that is undergoing continuous selective measurement of position. If the state of the system at a time t is given by the state vector $|\psi(t)\rangle$ then after a time τ ,

$$|\psi(t)\rangle \rightarrow |\psi(t+\tau)\rangle = \frac{\hat{U}\hat{M}_{\bar{x}}|\psi(t)\rangle}{\sqrt{\langle\psi(t)|\hat{M}_{\bar{x}}^\dagger\hat{M}_{\bar{x}}|\psi(t)\rangle}} = \frac{\hat{U}\hat{M}_{\bar{x}}|\psi(t)\rangle}{\sqrt{p_\psi(\bar{x})}}. \quad (3.47)$$

We now take the same approach as in the previous section where we evaluated the measurement part first in order to simplify the derivation. The quantities \hat{U} , $\hat{M}_{\bar{x}}$ and $p_\psi(\bar{x})$ are the same as those given in equations (3.7), (3.8) and (3.30) respectively. We evaluate the normalization in equation (3.47) as follows:

$$\begin{aligned} \frac{1}{\sqrt{p_\psi(\bar{x})}} &\approx \frac{1}{\sqrt{\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{\bar{x}^2}{2\sigma^2}\right) \left(1 + \frac{\bar{x}}{\sigma^2} \langle\hat{x}\rangle_\psi\right)}} \\ &= \sqrt[4]{2\pi\sigma^2} \exp\left(\frac{\bar{x}^2}{4\sigma^2}\right) \frac{1}{\sqrt{\left(1 + \frac{\bar{x}}{\sigma^2} \langle\hat{x}\rangle_\psi\right)}} \\ &\approx \sqrt[4]{2\pi\sigma^2} \exp\left(\frac{\bar{x}^2}{4\sigma^2}\right) \left(1 - \frac{\bar{x}}{2\sigma^2} \langle\hat{x}\rangle_\psi + \frac{3\bar{x}^2}{8\sigma^4} \langle\hat{x}\rangle_\psi^2\right). \end{aligned} \quad (3.48)$$

This in turn implies that

$$\begin{aligned} &\frac{\hat{M}_{\bar{x}}|\psi(t)\rangle}{\sqrt{p_\psi(\bar{x})}} \\ &= \left(1 - \frac{\bar{x}}{2\sigma^2} \langle\hat{x}\rangle_\psi + \frac{3\bar{x}^2}{8\sigma^4} \langle\hat{x}\rangle_\psi^2\right) \left(\mathbb{1} - \frac{\hat{x}^3\bar{x}}{8\sigma^4} + \frac{\hat{x}^2\bar{x}^2}{8\sigma^4} + \frac{\hat{x}\bar{x}}{2\sigma^2} + \frac{\hat{x}^4}{32\sigma^4} - \frac{\hat{x}^2}{4\sigma^2} + \mathcal{O}(\sigma^{-6})\right) |\psi(t)\rangle. \end{aligned} \quad (3.49)$$

Applying the Barchielli limit to (3.49), we obtain

$$\begin{aligned} \frac{\hat{M}_{\bar{x}}|\psi(t)\rangle}{\sqrt{p_\psi(\bar{x})}} &= \left(1 - \frac{\tau\gamma\bar{x}}{2} \langle\hat{x}\rangle_\psi + \frac{3\tau^2\gamma^2\bar{x}^2}{8} \langle\hat{x}\rangle_\psi^2\right) \\ &\times \left(\mathbb{1} - \frac{\tau^2\gamma^2\hat{x}^3\bar{x}}{8} + \frac{\tau^2\gamma^2\hat{x}^2\bar{x}^2}{8} + \frac{\tau\gamma\hat{x}\bar{x}}{2} + \frac{\tau^2\gamma^2\hat{x}^4}{32} - \frac{\tau\gamma\hat{x}^2}{4}\right) |\psi(t)\rangle. \end{aligned} \quad (3.50)$$

Substituting dQ for $\tau\bar{x}$ and subsequently applying Itô rules to equation (3.50), we get

$$\begin{aligned}
\frac{\hat{M}_{\bar{x}}|\psi(t)\rangle}{\sqrt{p_{\psi}(\bar{x})}} &= \left(1 - \frac{\gamma(dQ)}{2}\langle\hat{x}\rangle_{\psi} + \frac{3\gamma^2(dQ)^2}{8}\langle\hat{x}\rangle_{\psi}^2\right) \\
&\quad \times \left(\mathbb{1} - \frac{\tau\gamma^2(dQ)\hat{x}^3}{8} + \frac{\gamma^2(dQ)^2\hat{x}^2}{8} + \frac{\gamma(dQ)\hat{x}}{2} + \frac{\tau^2\gamma^2\hat{x}^4}{32} - \frac{\tau\gamma\hat{x}^2}{4}\right)|\psi(t)\rangle \\
&= \left(1 - \frac{\gamma(dQ)}{2}\langle\hat{x}\rangle_{\psi} + \frac{3\tau\gamma}{8}\langle\hat{x}\rangle_{\psi}^2\right)\left(\mathbb{1} + \frac{\tau\gamma\hat{x}^2}{8} + \frac{\gamma(dQ)\hat{x}}{2} - \frac{\tau\gamma\hat{x}^2}{4}\right)|\psi(t)\rangle \\
&= \left(1 - \frac{\gamma(dQ)}{2}\langle\hat{x}\rangle_{\psi} + \frac{3\tau\gamma}{8}\langle\hat{x}\rangle_{\psi}^2\right)\left(\mathbb{1} - \frac{\tau\gamma\hat{x}^2}{8} + \frac{\gamma(dQ)\hat{x}}{2}\right)|\psi(t)\rangle \\
&= \left(\mathbb{1} - \frac{\tau\gamma\hat{x}^2}{8} + \frac{\gamma(dQ)\hat{x}}{2} + \frac{3\tau\gamma}{8}\langle\hat{x}\rangle_{\psi}^2 - \frac{\gamma(dQ)}{2}\langle\hat{x}\rangle_{\psi} - \frac{\tau\gamma\hat{x}}{4}\langle\hat{x}\rangle_{\psi}\right)|\psi(t)\rangle \\
&= \left(\mathbb{1} - \frac{\tau\gamma\hat{x}^2}{8} + \frac{\tau\gamma\hat{x}}{4}\langle\hat{x}\rangle_{\psi} - \frac{\tau\gamma}{8}\langle\hat{x}\rangle_{\psi}^2 + \frac{\gamma(dQ)\hat{x}}{2}\right. \\
&\quad \left.- \frac{\gamma(dQ)}{2}\langle\hat{x}\rangle_{\psi} + \frac{\tau\gamma}{2}\langle\hat{x}\rangle_{\psi}^2 - \frac{\tau\gamma\hat{x}}{2}\langle\hat{x}\rangle_{\psi}\right)|\psi(t)\rangle \\
&= \left(\mathbb{1} - \frac{\tau\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_{\psi})^2 + \frac{\gamma(dQ)}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi}) - \frac{\tau\gamma}{2}\langle\hat{x}\rangle_{\psi}(\hat{x} - \langle\hat{x}\rangle_{\psi})\right)|\psi(t)\rangle \\
&= \left(\mathbb{1} - \frac{\tau\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_{\psi})^2 + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi})(dQ - \tau\langle\hat{x}\rangle_{\psi})\right)|\psi(t)\rangle. \tag{3.51}
\end{aligned}$$

Substituting equations (3.7) and (3.51) into (3.47), we obtain

$$\begin{aligned}
|\psi(t+\tau)\rangle &= \left(\mathbb{1} - \frac{i}{\hbar}\hat{H}\tau\right)\left(\mathbb{1} - \frac{\tau\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_{\psi})^2 + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi})(dQ - \tau\langle\hat{x}\rangle_{\psi})\right)|\psi(t)\rangle \\
&= \left(\mathbb{1} - \frac{i}{\hbar}\hat{H}\tau - \frac{\tau\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_{\psi})^2 + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi})(dQ - \tau\langle\hat{x}\rangle_{\psi})\right)|\psi(t)\rangle \\
\Rightarrow \Delta|\psi(t)\rangle &= \left(-\frac{i}{\hbar}\hat{H}\tau - \frac{\tau\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_{\psi})^2 + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi})(dQ - \tau\langle\hat{x}\rangle_{\psi})\right)|\psi(t)\rangle. \tag{3.52}
\end{aligned}$$

For an infinitesimal increment of the time dt , $\Delta|\psi(t)\rangle$ becomes $d|\psi(t)\rangle$ and therefore equation (3.52) becomes,

$$\begin{aligned}
d|\psi(t)\rangle &= \left(-\frac{i}{\hbar}\hat{H}dt - \frac{\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_{\psi})^2dt + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi})(dQ - \langle\hat{x}\rangle_{\psi}dt)\right)|\psi(t)\rangle \\
&= \left(\left(-\frac{i}{\hbar}\hat{H} - \frac{\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_{\psi})^2\right)dt + \frac{\sqrt{\gamma}}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi})dW\right)|\psi(t)\rangle, \tag{3.53}
\end{aligned}$$

which is the Itô stochastic Schrödinger equation for continuous position measurement.

3.5 Deduction of the stochastic master equation from the stochastic Schrödinger equation

In this section we show how to deduce the stochastic master equation from a given Itô stochastic Schrödinger equation. We start with the following Itô stochastic Schrödinger equation:

$$d|\psi(t)\rangle = \left(-\frac{i}{\hbar}\hat{H}dt - \frac{\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_\psi)^2dt + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_\psi)(dQ - \langle\hat{x}\rangle_\psi dt) \right) |\psi(t)\rangle. \quad (3.54)$$

For pure states the density operator

$$\hat{\rho}(t) = |\psi(t)\rangle\langle\psi(t)|, \quad (3.55)$$

implying that

$$d\hat{\rho}(t) = (d|\psi(t)\rangle)\langle\psi(t)| + |\psi(t)\rangle(d\langle\psi(t)|) + d|\psi(t)\rangle d\langle\psi(t)|. \quad (3.56)$$

It is important to note that we cannot ignore the $d|\psi(t)\rangle d\langle\psi(t)|$ term in equation (3.56) since terms containing $(dW)^2$ do not vanish according to Itô rules. To simplify calculations we abbreviate equation (3.54) as follows:

$$d|\psi(t)\rangle = \hat{B}|\psi(t)\rangle, \quad (3.57)$$

where

$$\hat{B} = \left(-\frac{i}{\hbar}\hat{H} - \frac{\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_\psi)^2 \right)dt + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_\psi)(dQ - \langle\hat{x}\rangle_\psi dt). \quad (3.58)$$

This in turn implies that

$$\hat{B}^\dagger = \left(\frac{i}{\hbar}\hat{H} - \frac{\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_\psi)^2 \right)dt + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_\psi)(dQ - \langle\hat{x}\rangle_\psi dt). \quad (3.59)$$

The operator \hat{B} is neither self-adjoint, as can be deduced from equations (3.58) and (3.59) nor unitary since

$$\hat{B}^\dagger \hat{B} = \hat{B} \hat{B}^\dagger = \frac{\gamma}{4}(\hat{x} - \langle\hat{x}\rangle)^2 dt. \quad (3.60)$$

Substituting equation (3.57) into equation (3.56), we obtain

$$d\hat{\rho}(t) = \hat{B}\hat{\rho}(t) + \hat{\rho}(t)\hat{B}^\dagger + \hat{B}\hat{\rho}(t)\hat{B}^\dagger. \quad (3.61)$$

Evaluating each term on the right hand side of equation (3.61) we obtain:

$$\hat{B}\hat{\rho}(t) = -\frac{i}{\hbar}\hat{H}\hat{\rho}(t)dt - \frac{\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_\psi)^2\hat{\rho}(t)dt + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_\psi)\hat{\rho}(dQ - \langle\hat{x}\rangle_\psi dt), \quad (3.62)$$

$$\hat{\rho}(t)\hat{B}^\dagger = \frac{i}{\hbar}\hat{\rho}(t)\hat{H}dt - \frac{\gamma}{8}\hat{\rho}(\hat{x} - \langle\hat{x}\rangle_\psi)^2dt + \frac{\gamma}{2}\hat{\rho}(\hat{x} - \langle\hat{x}\rangle_\psi)(dQ - \langle\hat{x}\rangle_\psi dt) \quad (3.63)$$

and

$$\hat{B}\hat{\rho}(t)\hat{B}^\dagger = \frac{\gamma}{4}\hat{x}\hat{\rho}(t)\hat{x}dt - \frac{\gamma}{4}\langle\hat{x}\rangle_\psi\hat{x}\hat{\rho}(t)dt - \frac{\gamma}{4}\langle\hat{x}\rangle_\psi\hat{\rho}(t)\hat{x}dt + \frac{\gamma}{4}\langle\hat{x}\rangle_\psi^2\hat{\rho}(t)dt. \quad (3.64)$$

Substituting equations (3.62), (3.63) and (3.64) into equation (3.61) yields the following:

$$\begin{aligned} d\hat{\rho}(t) &= -\frac{i}{\hbar}\hat{H}\hat{\rho}(t)dt + \frac{i}{\hbar}\hat{\rho}(t)\hat{H}dt + \frac{\gamma}{2}\hat{\rho}(\hat{x} - \langle\hat{x}\rangle_\psi)(dQ - \langle\hat{x}\rangle_\psi dt) \\ &\quad + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_\psi)\hat{\rho}(dQ - \langle\hat{x}\rangle_\psi dt) - \frac{\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_\psi)^2\hat{\rho}(t)dt - \frac{\gamma}{8}\hat{\rho}(\hat{x} - \langle\hat{x}\rangle_\psi)^2dt \\ &\quad + \frac{\gamma}{4}\hat{x}\hat{\rho}(t)\hat{x}dt - \frac{\gamma}{4}\langle\hat{x}\rangle_\psi\hat{x}\hat{\rho}(t)dt - \frac{\gamma}{4}\langle\hat{x}\rangle_\psi\hat{\rho}(t)\hat{x}dt + \frac{\gamma}{4}\langle\hat{x}\rangle_\psi^2\hat{\rho}(t)dt \\ &= -\frac{i}{\hbar}[\hat{H}, \hat{\rho}(t)]dt + \frac{\gamma}{2}\{\hat{x} - \langle\hat{x}\rangle_\psi, \hat{\rho}(t)\}(dQ - \langle\hat{x}\rangle_\psi dt) \\ &\quad - \frac{\gamma}{8}\hat{x}^2\hat{\rho}(t)dt - \frac{\gamma}{8}\hat{\rho}(t)\hat{x}^2dt + \frac{\gamma}{4}\hat{x}\hat{\rho}(t)\hat{x}dt \\ &= -\frac{i}{\hbar}[\hat{H}, \hat{\rho}(t)]dt - \frac{\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}(t)]]dt + \frac{\gamma}{2}\{\hat{x} - \langle\hat{x}\rangle_\psi, \hat{\rho}(t)\}(dQ - \langle\hat{x}\rangle_\psi dt), \end{aligned} \quad (3.65)$$

which is the master equation. The master equation preserves the pure state property $\hat{\rho}^2 = \hat{\rho}$. This was highlighted by Diósi [14]. The pure state property implies that for the state change

$$\hat{\rho} + d\hat{\rho} = (\hat{\rho} + d\hat{\rho})^2 = \hat{\rho}^2 + \hat{\rho}(d\hat{\rho}) + (d\hat{\rho})\hat{\rho} + d\hat{\rho}d\hat{\rho}. \quad (3.66)$$

From equation (3.66), it follows that we need to prove that

$$d\hat{\rho} = \hat{\rho}(d\hat{\rho}) + (d\hat{\rho})\hat{\rho} + d\hat{\rho}d\hat{\rho}. \quad (3.67)$$

The left hand side of equation (3.67) is given by equation (3.65). We now evaluate the terms on the right hand side as follows:

$$\begin{aligned} \hat{\rho}(d\hat{\rho}) &= -\frac{i}{\hbar}dt \underbrace{(\hat{\rho}\hat{H}\hat{\rho} - \hat{\rho}^2\hat{H})}_{\langle\hat{H}\rangle_{\hat{\rho}}\hat{\rho} - \hat{\rho}^2\hat{H}} - \frac{\gamma}{8}dt \left(\underbrace{\hat{\rho}\hat{x}^2\hat{\rho}}_{\langle\hat{x}^2\rangle_{\hat{\rho}}\hat{\rho}} + \underbrace{\hat{\rho}^2\hat{x}^2}_{\hat{\rho}\hat{x}^2} - 2\underbrace{\hat{\rho}\hat{x}\hat{\rho}\hat{x}}_{\langle\hat{x}\rangle_{\hat{\rho}}\hat{\rho}\hat{x}} \right) \\ &\quad + \frac{\gamma}{2}(dQ - \langle\hat{x}\rangle_{\hat{\rho}}dt) \underbrace{(\hat{\rho}\hat{x}\hat{\rho} + \hat{\rho}^2\hat{x} - 2\langle\hat{x}\rangle_{\hat{\rho}}\hat{\rho}^2)}_{\langle\hat{x}\rangle_{\hat{\rho}}\hat{\rho} + \hat{\rho}\hat{x} - 2\langle\hat{x}\rangle_{\hat{\rho}}\hat{\rho}}, \end{aligned} \quad (3.68)$$

$$\begin{aligned} (d\hat{\rho})\hat{\rho} &= -\frac{i}{\hbar}dt \underbrace{(\hat{H}\hat{\rho}^2 - \hat{\rho}\hat{H}\hat{\rho})}_{\hat{H}\hat{\rho} - \langle\hat{H}\rangle_{\hat{\rho}}\hat{\rho}} - \frac{\gamma}{8}dt \left(\underbrace{\hat{\rho}\hat{x}^2\hat{\rho}}_{\langle\hat{x}^2\rangle_{\hat{\rho}}\hat{\rho}} + \underbrace{\hat{x}^2\hat{\rho}^2}_{\hat{x}^2\hat{\rho}} - 2\underbrace{\hat{x}\hat{\rho}\hat{x}\hat{\rho}}_{\langle\hat{x}\rangle_{\hat{\rho}}\hat{\rho}\hat{x}} \right) \\ &\quad + \frac{\gamma}{2}(dQ - \langle\hat{x}\rangle_{\hat{\rho}}dt) \underbrace{(\hat{\rho}\hat{x}\hat{\rho} + \hat{x}\hat{\rho}^2 - 2\langle\hat{x}\rangle_{\hat{\rho}}\hat{\rho}^2)}_{\langle\hat{x}\rangle_{\hat{\rho}}\hat{\rho} + \hat{x}\hat{\rho} - 2\langle\hat{x}\rangle_{\hat{\rho}}\hat{\rho}}, \end{aligned} \quad (3.69)$$

$$\begin{aligned}
d\hat{\rho}d\hat{\rho} = & \frac{\gamma}{4} dt \overbrace{\left(\hat{x}\hat{\rho}\hat{x}\hat{\rho} + \hat{x}\hat{\rho}^2\hat{x} - 2\langle\hat{x}\rangle_{\hat{\rho}}\hat{x}\hat{\rho}^2 + \hat{\rho}\hat{x}^2\hat{\rho} + \hat{\rho}\hat{x}\hat{\rho}\hat{x} - 2\langle\hat{x}\rangle_{\hat{\rho}}\hat{\rho}\hat{x}\hat{\rho} \right.}^{\langle\hat{x}\rangle_{\hat{\rho}}\hat{x}\hat{\rho} + \hat{x}\hat{\rho}\hat{x} - 2\langle\hat{x}\rangle_{\hat{\rho}}\hat{x}\hat{\rho} + \langle\hat{x}^2\rangle_{\hat{\rho}}\hat{\rho} + \langle\hat{x}\rangle_{\hat{\rho}}\hat{\rho}\hat{x} - 2\langle\hat{x}\rangle_{\hat{\rho}}^2\hat{\rho}} \\
& \left. - 2\langle\hat{x}\rangle_{\hat{\rho}}\hat{\rho}\hat{x}\hat{\rho} - 2\langle\hat{x}\rangle_{\hat{\rho}}\hat{\rho}^2\hat{x} + 4\langle\hat{x}\rangle_{\hat{\rho}}^2\hat{\rho}^2 \right) \underbrace{\quad}_{-2\langle\hat{x}\rangle_{\hat{\rho}}^2\hat{\rho} - 2\langle\hat{x}\rangle_{\hat{\rho}}\hat{\rho}\hat{x} + 4\langle\hat{x}\rangle_{\hat{\rho}}^2\hat{\rho}}. \tag{3.70}
\end{aligned}$$

We now sum up equations (3.68), (3.69) and (3.70) to obtain

$$\begin{aligned}
\hat{\rho}(d\hat{\rho}) + (d\hat{\rho})\hat{\rho} + d\hat{\rho}d\hat{\rho} = & -\frac{i}{\hbar}(\hat{H}\hat{\rho} - \hat{\rho}\hat{H})dt - \frac{\gamma}{8}(\hat{\rho}\hat{x}^2 + \hat{x}^2\hat{\rho} - 2\hat{x}\hat{\rho}\hat{x})dt \\
& + \frac{\gamma}{2}(dQ - \langle\hat{x}\rangle_{\hat{\rho}}dt)(\hat{x}\hat{\rho} + \hat{\rho}\hat{x} - 2\langle\hat{x}\rangle_{\hat{\rho}}\hat{\rho}) \\
= & -\frac{i}{\hbar}[\hat{H}, \hat{\rho}]dt - \frac{\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}]]dt + \frac{\gamma}{2}(dQ - \langle\hat{x}\rangle_{\hat{\rho}}dt)\{\hat{x} - \langle\hat{x}\rangle_{\hat{\rho}}, \hat{\rho}\} \\
= & d\hat{\rho}. \tag{3.71}
\end{aligned}$$

3.6 Summary

In this chapter we showed that one can derive the equations of motion governing the evolution of the state of a quantum system whose position is continuously being observed by considering an experiment in which a sequence of unsharp position measurements, represented by positive operator valued measures, is performed in the Barchielli limit. We presented straight forward methods to derive the master equations for continuous measurement of position in both the selective and non-selective regimes, as well as the stochastic Schrödinger equation. To derive both the stochastic master equation and stochastic Schrödinger equation, one only need to apply the stochastic calculus, which was suggested by Diósi [14]. We also showed that given the stochastic Schrödinger equation, one can deduce the corresponding master equation, and that the stochastic master equation preserves the pure state condition.

Chapter 4

Monitoring the state of an individual quantum system

4.1 Introduction

In 2006 Diósi and his co-authors [15] introduced the concept of estimating the state of a quantum system, which is undergoing continuous selective measurement by means of a stochastic differential equation, which would be updated by the results of the measurement of the state of the system. The evolution of the estimated state would then be simulated numerically in a computer. Therefore, the scheme introduced in [15] can be used to monitor the state of the quantum system in real time. The ability to monitor the state of a quantum system makes it possible to control the state of the system in the sense that we can always apply unitary transformations to drive the system state to a desired one. In Chapter 3 we presented a new technique to derive both the master equation and the stochastic Schrödinger equation for continuous measurement of position. In this Chapter we apply the same technique to derive the master equation as well as the stochastic Schrödinger equation for the evolution of the estimated state. We explicitly derive both the stochastic master equation and the stochastic Schrödinger equation for the estimation of position as a way to show that with the new derivation technique one does not need to know special tricks like the ones in [15] to derive the equations.

4.2 Stochastic Master Equation for Continuous Position Estimation

We represent measurements by the same Kraus operators $\hat{M}_{\bar{x}}$ as in Chapter 3. The estimated wave function evolves in a similar fashion as the real one. The only difference is that it is updated using measurement results from the true wave function. If, at a time t , we estimate the state of our system

with the density operator $\hat{\rho}^e(t)$ then after a time τ

$$\hat{\rho}^e(t) \rightarrow \hat{\rho}^e(t + \tau) = \frac{1}{p_{\hat{\rho}^e}(\bar{x})} \hat{U} \hat{M}_{\bar{x}} \hat{\rho}^e(t) \hat{M}_{\bar{x}}^\dagger \hat{U}^\dagger, \quad (4.1)$$

where $p_{\hat{\rho}^e}(\bar{x})$ cannot be interpreted as the probability of obtaining the measurement result \bar{x} , but normalization, and is given by:

$$\begin{aligned} p_{\hat{\rho}^e}(\bar{x}) &= \text{tr} \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{(\hat{x} - \bar{x})^2}{2\sigma^2} \right) \hat{\rho}^e(t) \right\} \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \text{tr} \left\{ \exp \left(-\frac{\hat{x}^2 - 2\bar{x}\hat{x} + \bar{x}^2}{2\sigma^2} \right) \hat{\rho}^e(t) \right\} \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{\bar{x}^2}{2\sigma^2} \right) \text{tr} \left\{ \exp \left(-\frac{\hat{x}^2 - 2\bar{x}\hat{x}}{2\sigma^2} \right) \hat{\rho}^e(t) \right\} \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{\bar{x}^2}{2\sigma^2} \right) \text{tr} \left\{ \left(\mathbb{1} - \frac{\hat{x}^2 - 2\bar{x}\hat{x}}{2\sigma^2} + \frac{1}{2!} \left(-\frac{\hat{x}^2 - 2\bar{x}\hat{x}}{2\sigma^2} \right)^2 + \mathcal{O}(\sigma^{-6}) \right) \hat{\rho}^e(t) \right\} \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{\bar{x}^2}{2\sigma^2} \right) \text{tr} \left\{ \left(\mathbb{1} + \frac{\bar{x}}{\sigma^2} \hat{x} - \underbrace{\left(\frac{1}{2\sigma^2} - \frac{\bar{x}^2}{2\sigma^4} \right)}_{=0 \text{ in the limit}} \hat{x}^2 \right. \right. \\ &\quad \left. \left. - \frac{\bar{x}}{2\sigma^4} \hat{x}^3 + \frac{1}{8\sigma^4} \hat{x}^4 + \mathcal{O}(\sigma^{-6}) \right) \hat{\rho}^e(t) \right\} \\ &\quad \underbrace{\left(-\frac{\bar{x}}{2\sigma^4} \hat{x}^3 + \frac{1}{8\sigma^4} \hat{x}^4 + \mathcal{O}(\sigma^{-6}) \right)}_{\text{vanish in the limit}} \\ &\approx \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{\bar{x}^2}{2\sigma^2} \right) \left(\text{tr} \left\{ \hat{\rho}^e(t) \right\} + \text{tr} \left\{ \frac{\bar{x}\hat{x}}{\sigma^2} \hat{\rho}^e(t) \right\} \right) \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{\bar{x}^2}{2\sigma^2} \right) \left(1 + \frac{\bar{x}}{\sigma^2} \langle \hat{x} \rangle_{\hat{\rho}^e} \right). \end{aligned} \quad (4.2)$$

The quantity $\frac{1}{p_{\hat{\rho}^e}(\bar{x})}$ in equation (4.1) is given by

$$\frac{1}{p_{\hat{\rho}^e}(\bar{x})} \approx \sqrt{2\pi\sigma^2} \exp \left(\frac{\bar{x}^2}{2\sigma^2} \right) \left(1 - \frac{\bar{x}}{\sigma^2} \langle \hat{x} \rangle_{\hat{\rho}^e} + \frac{\bar{x}^2}{\sigma^4} \langle \hat{x} \rangle_{\hat{\rho}^e}^2 \right), \quad (4.3)$$

after applying a series expansion on the right hand side of the inverse of equation (4.2). Similarly, the measurement operators can be expanded as follows:

$$\begin{aligned} \hat{M}_{\bar{x}} &= \frac{1}{\sqrt{4\pi\sigma^2}} \exp \left(-\frac{(\hat{x} - \bar{x})^2}{4\sigma^2} \right) \\ &= \frac{1}{\sqrt{4\pi\sigma^2}} \exp \left(-\frac{\bar{x}^2}{4\sigma^2} \right) \exp \left(\frac{-\hat{x}^2 + 2\bar{x}\hat{x}}{4\sigma^2} \right) \\ &= \frac{1}{\sqrt{4\pi\sigma^2}} \exp \left(-\frac{\bar{x}^2}{4\sigma^2} \right) \left(\mathbb{1} - \frac{\hat{x}^3\bar{x}}{8\sigma^4} + \frac{\hat{x}^2\bar{x}^2}{8\sigma^4} + \frac{\hat{x}\bar{x}}{2\sigma^2} + \frac{\hat{x}^4}{32\sigma^4} - \frac{\hat{x}^2}{4\sigma^2} + \mathcal{O}(\sigma^{-6}) \right). \end{aligned} \quad (4.4)$$

To simplify the evaluation of equation (4.1), we first simplify the measurement part,

$$\frac{1}{p_{\hat{\rho}^e}(\bar{x})} \hat{M}_{\bar{x}} \hat{\rho}^e(t) \hat{M}_{\bar{x}}^\dagger,$$

by substituting equations (4.3) and (4.4) and obtain

$$\begin{aligned} & \frac{\hat{M}_{\bar{x}} \hat{\rho}^e(t) \hat{M}_{\bar{x}}^\dagger}{p_{\hat{\rho}^e}(\bar{x})} \\ &= \left(1 - \frac{\bar{x}}{\sigma^2} \langle \hat{x} \rangle_{\hat{\rho}^e} + \frac{\bar{x}^2}{\sigma^4} \langle \hat{x}^2 \rangle_{\hat{\rho}^e}\right) \left(1 - \frac{\hat{x}^3 \bar{x}}{8\sigma^4} + \frac{\hat{x}^2 \bar{x}^2}{8\sigma^4} + \frac{\hat{x} \bar{x}}{2\sigma^2} + \frac{\hat{x}^4}{32\sigma^4} - \frac{\hat{x}^2}{4\sigma^2} + \mathcal{O}(\sigma^{-6})\right) \hat{\rho}^e(t) \\ & \quad \times \left(1 - \frac{\hat{x}^3 \bar{x}}{8\sigma^4} + \frac{\hat{x}^2 \bar{x}^2}{8\sigma^4} + \frac{\hat{x} \bar{x}}{2\sigma^2} + \frac{\hat{x}^4}{32\sigma^4} - \frac{\hat{x}^2}{4\sigma^2} + \mathcal{O}(\sigma^{-6})\right) \\ &= \left(1 - \frac{\bar{x}}{\sigma^2} \langle \hat{x} \rangle_{\hat{\rho}^e} + \frac{\bar{x}^2}{\sigma^4} \langle \hat{x}^2 \rangle_{\hat{\rho}^e}\right) \left(\hat{\rho}^e(t) + \frac{\bar{x}}{2\sigma^2} \hat{x} \hat{\rho}^e(t) + \frac{\bar{x}}{2\sigma^2} \hat{\rho}^e(t) \hat{x} - \frac{1}{4\sigma^2} \hat{x}^2 \hat{\rho}^e(t) - \frac{1}{4\sigma^2} \hat{\rho}^e(t) \hat{x}^2 \right. \\ & \quad + \frac{\bar{x}^2}{8\sigma^4} \hat{x}^2 \hat{\rho}^e(t) + \frac{\bar{x}^2}{8\sigma^4} \hat{\rho}^e(t) \hat{x}^2 + \frac{\bar{x}^2}{4\sigma^4} \hat{x} \hat{\rho}^e(t) \hat{x} - \frac{\bar{x}}{8\sigma^4} \hat{x}^3 \hat{\rho}^e(t) - \frac{\bar{x}}{8\sigma^4} \hat{\rho}^e(t) \hat{x}^3 \\ & \quad + \frac{1}{32\sigma^4} \hat{x}^4 \hat{\rho}^e(t) + \frac{1}{32\sigma^4} \hat{\rho}^e(t) \hat{x}^4 - \frac{\bar{x}}{4\sigma^4} \hat{x}^2 \hat{\rho}^e(t) \hat{x} + \frac{1}{16\sigma^4} \hat{x}^2 \hat{\rho}^e(t) \hat{x}^2 + \mathcal{O}(\sigma^{-6}) \Big) \\ &= \left(1 - \frac{\bar{x}}{\sigma^2} \langle \hat{x} \rangle_{\hat{\rho}^e} + \frac{\bar{x}^2}{\sigma^4} \langle \hat{x}^2 \rangle_{\hat{\rho}^e}\right) \left(\hat{\rho}^e(t) + \frac{\bar{x}}{2\sigma^2} \{\hat{x}, \hat{\rho}^e(t)\} - \frac{1}{8\sigma^2} [\hat{x}, [\hat{x}, \hat{\rho}^e(t)]] - \frac{1}{8\sigma^2} \{\hat{x}, \{\hat{x}, \hat{\rho}^e(t)\}\} \right. \\ & \quad + \frac{\bar{x}^2}{8\sigma^4} \{\hat{x}, \{\hat{x}, \hat{\rho}^e(t)\}\} - \frac{\bar{x}}{8\sigma^4} \{\hat{x}^3, \hat{\rho}^e(t)\} + \frac{1}{32\sigma^4} \{\hat{x}^4, \hat{\rho}^e(t)\} \\ & \quad \left. - \frac{\bar{x}}{4\sigma^4} \hat{x}^2 \hat{\rho}^e(t) \hat{x} + \frac{1}{16\sigma^4} \hat{x}^2 \hat{\rho}^e(t) \hat{x}^2 + \mathcal{O}(\sigma^{-6}) \right). \end{aligned} \tag{4.5}$$

After applying the Barchielli limit, equation (4.5) becomes:

$$\begin{aligned} & \frac{\hat{M}_{\bar{x}} \hat{\rho}^e(t) \hat{M}_{\bar{x}}^\dagger}{p_{\hat{\rho}^e}(\bar{x})} \\ &= \left(1 - \bar{x} \tau \gamma \langle \hat{x} \rangle_{\hat{\rho}^e} + \bar{x}^2 \tau^2 \gamma^2 \langle \hat{x}^2 \rangle_{\hat{\rho}^e}\right) \left(\hat{\rho}^e(t) + \frac{\bar{x} \tau \gamma}{2} \{\hat{x}, \hat{\rho}^e(t)\} - \frac{\tau \gamma}{8} [\hat{x}, [\hat{x}, \hat{\rho}^e(t)]] \right. \\ & \quad - \frac{\tau \gamma}{8} \{\hat{x}, \{\hat{x}, \hat{\rho}^e(t)\}\} + \frac{\bar{x}^2 \tau^2 \gamma^2}{8} \{\hat{x}, \{\hat{x}, \hat{\rho}^e(t)\}\} - \frac{\bar{x} \tau^2 \gamma^2}{8} \{\hat{x}^3, \hat{\rho}^e(t)\} + \frac{\tau^2 \gamma^2}{32} \{\hat{x}^4, \hat{\rho}^e(t)\} \\ & \quad \left. - \frac{\bar{x} \tau^2 \gamma^2}{4} \hat{x}^2 \hat{\rho}^e(t) \hat{x} + \frac{\tau^2 \gamma^2}{16} \hat{x}^2 \hat{\rho}^e(t) \hat{x}^2 + \mathcal{O}(\sigma^{-6}) \right). \end{aligned} \tag{4.6}$$

In order for us to further simplify equation (4.6), we introduce the same stochastic quantity dQ as we did in Chapter 2. Substituting (dQ) for $\bar{x}\tau$ into equation (4.6) we obtain:

$$\begin{aligned}
& \frac{\hat{M}_{\bar{x}}\hat{\rho}^e(t)\hat{M}_{\bar{x}}^\dagger}{p_{\hat{\rho}^e}(\bar{x})} \\
&= \left(1 - (dQ)\gamma\langle\hat{x}\rangle_{\hat{\rho}^e} + (dQ)^2\gamma^2\langle\hat{x}\rangle_{\hat{\rho}^e}^2\right) \left(\hat{\rho}^e(t) + \frac{(dQ)\gamma}{2}\{\hat{x}, \hat{\rho}^e(t)\} - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}^e(t)]]\right. \\
&\quad - \frac{\tau\gamma}{8}\{\hat{x}, \{\hat{x}, \hat{\rho}^e(t)\}\} + \frac{(dQ)^2\gamma^2}{8}\{\hat{x}, \{\hat{x}, \hat{\rho}^e(t)\}\} - \frac{(dQ)\tau\gamma^2}{8}\{\hat{x}^3, \hat{\rho}^e(t)\} \\
&\quad \left. + \frac{\tau^2\gamma^2}{32}\{\hat{x}^4, \hat{\rho}^e(t)\} - \frac{(dQ)\tau\gamma^2}{4}\hat{x}^2\hat{\rho}^e(t)\hat{x} + \frac{\tau^2\gamma^2}{16}\hat{x}^2\hat{\rho}^e(t)\hat{x}^2 + \mathcal{O}(\sigma^{-6})\right). \tag{4.7}
\end{aligned}$$

We now apply Itô rules to equation (4.7). We therefore re-write equation (4.7) as follows:

$$\begin{aligned}
& \frac{\hat{M}_{\bar{x}}\hat{\rho}^e(t)\hat{M}_{\bar{x}}^\dagger}{p_{\hat{\rho}^e}(\bar{x})} \\
&= \left(1 - (dQ)\gamma\langle\hat{x}\rangle_{\hat{\rho}^e} + \tau\gamma\langle\hat{x}\rangle_{\hat{\rho}^e}^2\right) \left(\hat{\rho}^e(t) + \frac{(dQ)\gamma}{2}\{\hat{x}, \hat{\rho}^e(t)\} - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}^e(t)]]\right. \\
&\quad \left. - \frac{\tau\gamma}{8}\{\hat{x}, \{\hat{x}, \hat{\rho}^e(t)\}\} + \frac{\tau\gamma^2}{8\gamma}\{\hat{x}, \{\hat{x}, \hat{\rho}^e(t)\}\}\right) \\
&= \left(1 - (dQ)\gamma\langle\hat{x}\rangle_{\hat{\rho}^e} + \tau\gamma\langle\hat{x}\rangle_{\hat{\rho}^e}^2\right) \left(\hat{\rho}^e(t) + \frac{(dQ)\gamma}{2}\{\hat{x}, \hat{\rho}^e(t)\} - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}^e(t)]]\right) \\
&= \hat{\rho}^e(t) - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}^e(t)]] + \frac{(dQ)\gamma}{2}\{\hat{x}, \hat{\rho}^e(t)\} - (dQ)\gamma\hat{\rho}^e(t)\langle\hat{x}\rangle_{\hat{\rho}^e} \\
&\quad - \frac{\tau\gamma\langle\hat{x}\rangle_{\hat{\rho}^e}}{2}\{\hat{x}, \hat{\rho}^e(t)\} + \tau\gamma\langle\hat{x}\rangle_{\hat{\rho}^e}^2\hat{\rho}^e(t) \\
&= \hat{\rho}^e(t) - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}^e(t)]] + \frac{(dQ)\gamma}{2}\{\hat{x} - \langle\hat{x}\rangle_{\hat{\rho}^e}, \hat{\rho}^e(t)\} - \frac{\tau\gamma\langle\hat{x}\rangle_{\hat{\rho}^e}}{2}\{\hat{x} - \langle\hat{x}\rangle_{\hat{\rho}^e}, \hat{\rho}^e(t)\} \\
&= \hat{\rho}^e(t) - \frac{\tau\gamma}{8}[\hat{x}, [\hat{x}, \hat{\rho}^e(t)]] + \frac{\gamma}{2}\{\hat{x} - \langle\hat{x}\rangle_{\hat{\rho}^e}, \hat{\rho}^e(t)\}(dQ - \tau\langle\hat{x}\rangle_{\hat{\rho}^e}). \tag{4.8}
\end{aligned}$$

We now apply the unitary evolution to obtain

$$\begin{aligned}
& \hat{\rho}^e(t + \tau) \\
&= \frac{1}{p_{\hat{\rho}^e}(\bar{x})} \hat{U} \hat{M}_{\bar{x}} \hat{\rho}^e(t) \hat{M}_{\bar{x}}^\dagger \hat{U}^\dagger \\
&= \left(\mathbb{1} - \frac{i}{\hbar} \hat{H} \tau + \mathcal{O}(\tau^2) \right) \left(\hat{\rho}^e(t) - \frac{\tau \gamma}{8} [\hat{x}, [\hat{x}, \hat{\rho}^e(t)]] + \frac{\gamma}{2} \{ \hat{x} - \langle \hat{x} \rangle_{\hat{\rho}^e}, \hat{\rho}^e(t) \} (dQ - \tau \langle \hat{x} \rangle_{\hat{\rho}^e}) \right) \\
&\quad \times \left(\mathbb{1} + \frac{i}{\hbar} \hat{H} \tau + \mathcal{O}(\tau^2) \right) \\
&= \hat{\rho}^e(t) - \frac{\tau \gamma}{8} [\hat{x}, [\hat{x}, \hat{\rho}^e(t)]] + \frac{\gamma}{2} \{ \hat{x} - \langle \hat{x} \rangle_{\hat{\rho}^e}, \hat{\rho}^e(t) \} (dQ - \tau \langle \hat{x} \rangle_{\hat{\rho}^e}) - \frac{i}{\hbar} \hat{H} \tau \hat{\rho}^e(t) + \hat{\rho}^e(t) \frac{i}{\hbar} \hat{H} \tau \\
&= \hat{\rho}^e(t) - \frac{i \tau}{\hbar} [\hat{H}, \hat{\rho}^e(t)] - \frac{\tau \gamma}{8} [\hat{x}, [\hat{x}, \hat{\rho}^e(t)]] + \frac{\gamma}{2} \{ \hat{x} - \langle \hat{x} \rangle_{\hat{\rho}^e}, \hat{\rho}^e(t) \} (dQ - \tau \langle \hat{x} \rangle_{\hat{\rho}^e}). \tag{4.9}
\end{aligned}$$

For an infinitesimal time increment dt equation (4.9) reduces to

$$\begin{aligned}
d\hat{\rho}^e(t) &= -\frac{i}{\hbar} [\hat{H}, \hat{\rho}^e(t)] dt - \frac{\gamma}{8} [\hat{x}, [\hat{x}, \hat{\rho}^e(t)]] dt + \frac{\gamma}{2} \{ \hat{x} - \langle \hat{x} \rangle_{\hat{\rho}^e}, \hat{\rho}^e(t) \} (dQ - \langle \hat{x} \rangle_{\hat{\rho}^e} dt) \\
&= -\frac{i}{\hbar} [\hat{H}, \hat{\rho}^e(t)] dt - \frac{\gamma}{8} [\hat{x}, [\hat{x}, \hat{\rho}^e(t)]] dt + \frac{\gamma}{2} \{ \hat{x} - \langle \hat{x} \rangle_{\hat{\rho}^e}, \hat{\rho}^e(t) \} (\langle \hat{x} \rangle_{\hat{\rho}} - \langle \hat{x} \rangle_{\hat{\rho}^e}) dt \\
&\quad + \frac{\sqrt{\gamma}}{2} \{ \hat{x} - \langle \hat{x} \rangle_{\hat{\rho}^e}, \hat{\rho}^e(t) \} dW, \tag{4.10}
\end{aligned}$$

which is the master equation for continuous estimation of position in the selective regime.

4.3 Itô Stochastic Schrödinger Equation for Continuous Position Estimation

The stochastic Schrödinger equation of estimation is derived in a similar way as the one for measurement in Chapter 3. If the state of the system at a time t is given by $|\psi_e(t)\rangle$, then after a time τ the state of the system

$$|\psi_e(t)\rangle \rightarrow |\psi_e(t + \tau)\rangle = \frac{\hat{U} \hat{M}_{\bar{x}} |\psi_e(t)\rangle}{\sqrt{\langle \psi_e(t) | \hat{M}_{\bar{x}}^\dagger \hat{M}_{\bar{x}} | \psi_e(t) \rangle}} = \frac{\hat{U} \hat{M}_{\bar{x}} |\psi_e(t)\rangle}{\sqrt{p_{\psi_e}(\bar{x})}}. \tag{4.11}$$

We shall now take the same approach as in the previous section. We will evaluate the measurement part first in order to simplify the derivation. The quantities \hat{U} , $\hat{M}_{\bar{x}}$ and $p_{\psi_e}(\bar{x})$ are given in equations

(3.7), (4.4) and (4.3) respectively. We will now evaluate

$$\begin{aligned}
\frac{1}{\sqrt{p_{\psi_e}(\bar{x})}} &= \frac{1}{\sqrt{\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{\bar{x}^2}{2\sigma^2}\right) \left(1 + \frac{\bar{x}}{\sigma^2} \langle \hat{x} \rangle_{\psi_e}\right)}} \\
&= \sqrt[4]{2\pi\sigma^2} \exp\left(\frac{\bar{x}^2}{4\sigma^2}\right) \frac{1}{\sqrt{\left(1 + \frac{\bar{x}}{\sigma^2} \langle \hat{x} \rangle_{\psi_e}\right)}} \\
&= \sqrt[4]{2\pi\sigma^2} \exp\left(\frac{\bar{x}^2}{4\sigma^2}\right) \left(1 - \frac{\bar{x}}{2\sigma^2} \langle \hat{x} \rangle_{\psi_e} + \frac{3\bar{x}^2}{8\sigma^4} \langle \hat{x} \rangle_{\psi_e}^2\right). \tag{4.12}
\end{aligned}$$

In turn,

$$\begin{aligned}
&\frac{\hat{M}_{\bar{x}}|\psi_e(t)\rangle}{\sqrt{p_{\psi_e}(\bar{x})}} \\
&= \left(1 - \frac{\bar{x}}{2\sigma^2} \langle \hat{x} \rangle_{\psi_e} + \frac{3\bar{x}^2}{8\sigma^4} \langle \hat{x} \rangle_{\psi_e}^2\right) \left(\mathbb{1} - \frac{\hat{x}^3 \bar{x}}{8\sigma^4} + \frac{\hat{x}^2 \bar{x}^2}{8\sigma^4} + \frac{\hat{x} \bar{x}}{2\sigma^2} + \frac{\hat{x}^4}{32\sigma^4} - \frac{\hat{x}^2}{4\sigma^2} + \mathcal{O}(\sigma^{-6})\right) |\psi_e(t)\rangle. \tag{4.13}
\end{aligned}$$

Applying the Barchielli limit to (4.13), we obtain

$$\begin{aligned}
\frac{\hat{M}_{\bar{x}}|\psi_e(t)\rangle}{\sqrt{p_{\psi_e}(\bar{x})}} &= \left(1 - \frac{\tau\gamma\bar{x}}{2} \langle \hat{x} \rangle_{\psi_e} + \frac{3\tau^2\gamma^2\bar{x}^2}{8} \langle \hat{x} \rangle_{\psi_e}^2\right) \\
&\times \left(\mathbb{1} - \frac{\tau^2\gamma^2\hat{x}^3\bar{x}}{8} + \frac{\tau^2\gamma^2\hat{x}^2\bar{x}^2}{8} + \frac{\tau\gamma\hat{x}\bar{x}}{2} + \frac{\tau^2\gamma^2\hat{x}^4}{32} - \frac{\tau\gamma\hat{x}^2}{4}\right) |\psi_e(t)\rangle. \tag{4.14}
\end{aligned}$$

Substituting dQ for $\tau\bar{x}$ and subsequently applying Itô rules equation (4.14),

$$\begin{aligned}
\frac{\hat{M}_{\bar{x}}|\psi_e(t)\rangle}{\sqrt{p_{\psi_e}(\bar{x})}} &= \left(1 - \frac{\gamma(dQ)}{2}\langle\hat{x}\rangle_{\psi_e} + \frac{3\gamma^2(dQ)^2}{8}\langle\hat{x}\rangle_{\psi_e}^2\right) \\
&\quad \times \left(\mathbb{1} - \frac{\tau\gamma^2(dQ)\hat{x}^3}{8} + \frac{\gamma^2(dQ)^2\hat{x}^2}{8} + \frac{\gamma(dQ)\hat{x}}{2} + \frac{\tau^2\gamma^2\hat{x}^4}{32} - \frac{\tau\gamma\hat{x}^2}{4}\right)|\psi_e(t)\rangle \\
&= \left(1 - \frac{\gamma(dQ)}{2}\langle\hat{x}\rangle_{\psi_e} + \frac{3\tau\gamma}{8}\langle\hat{x}\rangle_{\psi_e}^2\right)\left(\mathbb{1} + \frac{\tau\gamma\hat{x}^2}{8} + \frac{\gamma(dQ)\hat{x}}{2} - \frac{\tau\gamma\hat{x}^2}{4}\right)|\psi_e(t)\rangle \\
&= \left(1 - \frac{\gamma(dQ)}{2}\langle\hat{x}\rangle_{\psi_e} + \frac{3\tau\gamma}{8}\langle\hat{x}\rangle_{\psi_e}^2\right)\left(\mathbb{1} - \frac{\tau\gamma\hat{x}^2}{8} + \frac{\gamma(dQ)\hat{x}}{2}\right)|\psi_e(t)\rangle \\
&= \left(\mathbb{1} - \frac{\tau\gamma\hat{x}^2}{8} + \frac{\gamma(dQ)\hat{x}}{2} + \frac{3\tau\gamma}{8}\langle\hat{x}\rangle_{\psi_e}^2 - \frac{\gamma(dQ)}{2}\langle\hat{x}\rangle_{\psi_e} - \frac{\tau\gamma\hat{x}}{4}\langle\hat{x}\rangle_{\psi_e}\right)|\psi_e(t)\rangle \\
&= \left(\mathbb{1} - \frac{\tau\gamma\hat{x}^2}{8} + \frac{\tau\gamma\hat{x}}{4}\langle\hat{x}\rangle_{\psi_e} - \frac{\tau\gamma}{8}\langle\hat{x}\rangle_{\psi_e}^2 + \frac{\gamma(dQ)\hat{x}}{2}\right. \\
&\quad \left.- \frac{\gamma(dQ)}{2}\langle\hat{x}\rangle_{\psi_e} + \frac{\tau\gamma}{2}\langle\hat{x}\rangle_{\psi_e}^2 - \frac{\tau\gamma\hat{x}}{2}\langle\hat{x}\rangle_{\psi_e}\right)|\psi_e(t)\rangle \\
&= \left(\mathbb{1} - \frac{\tau\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})^2 + \frac{\gamma(dQ)}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi_e}) - \frac{\tau\gamma}{2}\langle\hat{x}\rangle_{\psi_e}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})\right)|\psi_e(t)\rangle \\
&= \left(\mathbb{1} - \frac{\tau\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})^2 + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})(dQ - \tau\langle\hat{x}\rangle_{\psi_e})\right)|\psi_e(t)\rangle. \tag{4.15}
\end{aligned}$$

Substituting equations (3.7) and (4.15) into (4.11),

$$\begin{aligned}
|\psi_e(t + \tau)\rangle &= \left(\mathbb{1} - \frac{i}{\hbar}\hat{H}\tau\right)\left(\mathbb{1} - \frac{\tau\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})^2 + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})(dQ - \tau\langle\hat{x}\rangle_{\psi_e})\right)|\psi_e(t)\rangle \\
&= \left(\mathbb{1} - \frac{i}{\hbar}\hat{H}\tau - \frac{\tau\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})^2 + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})(dQ - \tau\langle\hat{x}\rangle_{\psi_e})\right)|\psi_e(t)\rangle \\
\Rightarrow \Delta|\psi_e(t)\rangle &= \left(-\frac{i}{\hbar}\hat{H}\tau - \frac{\tau\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})^2 + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})(dQ - \tau\langle\hat{x}\rangle_{\psi_e})\right)|\psi_e(t)\rangle. \tag{4.16}
\end{aligned}$$

For an infinitesimal increment of the time dt equation (4.16) reduces to

$$\begin{aligned}
d|\psi_e(t)\rangle &= \left(-\frac{i}{\hbar}\hat{H}dt - \frac{\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})^2dt + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})(dQ - \langle\hat{x}\rangle_{\psi_e}dt)\right)|\psi_e(t)\rangle \\
&= \left(\left(-\frac{i}{\hbar}\hat{H} - \frac{\gamma}{8}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})^2 + \frac{\gamma}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})(\langle\hat{x}\rangle_{\psi_e} - \langle\hat{x}\rangle_{\psi_e})\right)dt\right. \\
&\quad \left.+ \frac{\sqrt{\gamma}}{2}(\hat{x} - \langle\hat{x}\rangle_{\psi_e})dW\right)|\psi_e(t)\rangle, \tag{4.17}
\end{aligned}$$

which is the Itô stochastic Schrödinger equation for continuous position estimation.

4.4 Convergence

The theory of monitoring the state of a single system relies on the asymptotic convergence of the estimated state to the real one, in a reasonable finite time. To measure the convergence of the estimated state to the real one we calculate the Uhlmann fidelity [58], which tells us how well two quantum states overlap with each other. This fidelity is given by

$$F(\psi_1(x, t), \psi_2(x, t)) = \left| \int_{-\infty}^{\infty} \psi_1^*(x, t) \psi_2(x, t) dx \right|^2, \quad (4.18)$$

for two normalized wave functions $\psi_1(x, t) = \langle x | \psi_1(t) \rangle$ and $\psi_2(x, t) = \langle x | \psi_2(t) \rangle$, where $|x\rangle$ is an eigenstate of the position operator \hat{x} . In the density operator formalism, the fidelity between two states $\hat{\rho}_1(t)$ and $\hat{\rho}_2(t)$ is given by

$$F(\hat{\rho}_1(t), \hat{\rho}_2(t)) = \text{tr} \left\{ \sqrt{\sqrt{\hat{\rho}_1(t)} \hat{\rho}_2(t) \sqrt{\hat{\rho}_1(t)}} \right\}. \quad (4.19)$$

Uhlmann fidelity takes values in the range $[0, 1]$. We shall use the density operator formalism to argue that the estimated state $\hat{\rho}^e$ of the system, which evolves according to equation (4.10), converges to the real state $\hat{\rho}$ almost always. The proof of this convergence can be found in [15]. Below we shall point out the key components of the proof. Instead of using the fidelity measure given in (4.19), we can use the pure state condition, $\text{tr}\{\hat{\rho}^2\} = 1$, because the solutions $\hat{\rho}(t)$ of the master equation (3.46) for long times t are pure states, (see [18, 15]). From the pure state condition:

$$\text{tr}\{\hat{\rho}^2\} = 1, \quad (4.20)$$

we can deduce that

$$\text{tr}\{\hat{\rho}^e \hat{\rho}\} = 1, \quad (4.21)$$

implies that the two pure states $\hat{\rho}^e$ and $\hat{\rho}$ are equal, and

$$\text{tr}\{\hat{\rho}^e \hat{\rho}\} = 0, \quad (4.22)$$

implies that the two states have no overlap. Therefore the quantity $\text{tr}\{\hat{\rho}^e \hat{\rho}\}$ is bounded the same way as fidelity, which is defined by equation (4.19). To prove convergence it suffices to show that for different states $\hat{\rho}^e$ and $\hat{\rho}$, which are evolving according to equations (4.10) and (3.46) respectively,

$$d \left\langle \text{tr}\{\hat{\rho}^e \hat{\rho}\} \right\rangle_{st} \geq 0, \quad (4.23)$$

implying that the average overlap between the two states $\hat{\rho}^e$ and $\hat{\rho}$ monotonically increases until it asymptotically reaches unity. We now expand the left hand side of equation (4.23) as follows:

$$\begin{aligned} d\langle \text{tr}\{\hat{\rho}^e \hat{\rho}\} \rangle_{st} &= \langle \text{tr}\{d(\hat{\rho}^e \hat{\rho})\} \rangle_{st} \\ &= \langle \text{tr}\{d\hat{\rho}^e \hat{\rho} + \hat{\rho}^e d\hat{\rho} + d\hat{\rho}^e d\hat{\rho}\} \rangle_{st} \\ &= \langle \text{tr}\{d\hat{\rho}^e \hat{\rho}\} + \text{tr}\{\hat{\rho}^e d\hat{\rho}\} + \text{tr}\{d\hat{\rho}^e d\hat{\rho}\} \rangle_{st}. \end{aligned} \quad (4.24)$$

In order to simplify our calculations we will calculate the terms $\text{tr}\{d\hat{\rho}^e \hat{\rho}\}$, $\text{tr}\{\hat{\rho}^e d\hat{\rho}\}$, and $\text{tr}\{d\hat{\rho}^e d\hat{\rho}\}$ individually as follows:

$$\begin{aligned} \text{tr}\{d\hat{\rho}^e \hat{\rho}\} &= -\frac{i}{\hbar} dt [\text{tr}\{\hat{H} \hat{\rho}^e \hat{\rho}\} - \text{tr}\{\hat{H} \hat{\rho} \hat{\rho}^e\}] \\ &\quad - \frac{\gamma}{8} dt [\text{tr}\{\hat{x}^2 \hat{\rho}^e \hat{\rho}\} + \text{tr}\{\hat{x}^2 \hat{\rho} \hat{\rho}^e\} - 2 \text{tr}\{\hat{x} \hat{\rho}^e \hat{x} \hat{\rho}\}] \\ &\quad + \frac{\gamma}{2} dt (\langle x \rangle_{\hat{\rho}} - \langle x \rangle_{\hat{\rho}^e}) [\text{tr}\{\hat{x} \hat{\rho}^e \hat{\rho}\} + \text{tr}\{\hat{x} \hat{\rho} \hat{\rho}^e\} - 2 \langle x \rangle_{\hat{\rho}^e} \text{tr}\{\hat{\rho}^e \hat{\rho}\}] \\ &\quad + \frac{\sqrt{\gamma}}{2} dW [\text{tr}\{\hat{x} \hat{\rho}^e \hat{\rho}\} + \text{tr}\{\hat{x} \hat{\rho} \hat{\rho}^e\} - 2 \langle x \rangle_{\hat{\rho}^e} \text{tr}\{\hat{\rho}^e \hat{\rho}\}], \end{aligned} \quad (4.25)$$

$$\begin{aligned} \text{tr}\{\hat{\rho}^e d\hat{\rho}\} &= -\frac{i}{\hbar} dt [\text{tr}\{\hat{H} \hat{\rho} \hat{\rho}^e\} - \text{tr}\{\hat{H} \hat{\rho}^e \hat{\rho}\}] \\ &\quad - \frac{\gamma}{8} dt [\text{tr}\{\hat{x}^2 \hat{\rho}^e \hat{\rho}\} + \text{tr}\{\hat{x}^2 \hat{\rho} \hat{\rho}^e\} - 2 \text{tr}\{\hat{x} \hat{\rho}^e \hat{x} \hat{\rho}\}] \\ &\quad + \frac{\sqrt{\gamma}}{2} dW [\text{tr}\{\hat{x} \hat{\rho}^e \hat{\rho}\} + \text{tr}\{\hat{x} \hat{\rho} \hat{\rho}^e\} - 2 \langle x \rangle_{\hat{\rho}} \text{tr}\{\hat{\rho}^e \hat{\rho}\}] \end{aligned} \quad (4.26)$$

and

$$\begin{aligned} \text{tr}\{d\hat{\rho}^e d\hat{\rho}\} &= \frac{\gamma}{4} dt [2 \text{tr}\{\hat{x} \hat{\rho}^e \hat{x} \hat{\rho}\} - 2 (\langle x \rangle_{\hat{\rho}} + \langle x \rangle_{\hat{\rho}^e}) \text{tr}\{\hat{x} \hat{\rho}^e \hat{\rho}\} \\ &\quad - 2 (\langle x \rangle_{\hat{\rho}} + \langle x \rangle_{\hat{\rho}^e}) \text{tr}\{\hat{x} \hat{\rho} \hat{\rho}^e\} + 4 \langle \hat{x} \rangle_{\hat{\rho}^e} \langle \hat{x} \rangle_{\hat{\rho}} \text{tr}\{\hat{\rho}^e \hat{\rho}\} \\ &\quad + \text{tr}\{\hat{x}^2 \hat{\rho}^e \hat{\rho}\} + \text{tr}\{\hat{x}^2 \hat{\rho} \hat{\rho}^e\}]. \end{aligned} \quad (4.27)$$

Substituting equations (4.25), (4.26) and (4.27) into (4.24), we obtain

$$\begin{aligned}
d\langle \text{tr}\{\hat{\rho}^e \hat{\rho}\} \rangle_{st} &= \left\langle \frac{\gamma}{2} dt \left(\langle x \rangle_{\hat{\rho}} - \langle x \rangle_{\hat{\rho}^e} \right) \left[-2\langle x \rangle_{\hat{\rho}^e} \text{tr}\{\hat{\rho}^e \hat{\rho}\} \right] \right. \\
&\quad + \sqrt{\gamma} dW \left[\text{tr}\{\hat{x} \hat{\rho}^e \hat{\rho}\} + \text{tr}\{\hat{x} \hat{\rho} \hat{\rho}^e\} - 2\langle x \rangle_{\hat{\rho}^e} \text{tr}\{\hat{\rho}^e \hat{\rho}\} \right] \\
&\quad + \gamma dt \langle \hat{x} \rangle_{\hat{\rho}^e} \langle \hat{x} \rangle_{\hat{\rho}} \text{tr}\{\hat{\rho}^e \hat{\rho}\} + \gamma dt \text{tr}\{\hat{x} \hat{\rho}^e \hat{x} \hat{\rho}\} \\
&\quad \left. - \langle \hat{x} \rangle_{\hat{\rho}^e} \text{tr}\{\hat{x} \hat{\rho} \hat{\rho}^e + \hat{x} \hat{\rho}^e \hat{\rho}\} \right\rangle_{st} \\
&= \text{tr}\left\{ \hat{x} \hat{\rho}^e \hat{x} \hat{\rho} + \langle \hat{x} \rangle_{\hat{\rho}^e}^2 \hat{\rho}^e \hat{\rho} - \langle \hat{x} \rangle_{\hat{\rho}^e} (\hat{x} \hat{\rho} \hat{\rho}^e + \hat{x} \hat{\rho}^e \hat{\rho}) \right\} \\
&= \text{tr}\left\{ (\hat{x} - \langle \hat{x} \rangle_{\hat{\rho}^e}) \hat{\rho}^e (\hat{x} - \langle \hat{x} \rangle_{\hat{\rho}^e}) \hat{\rho} \right\} \\
&= \text{tr}\left\{ \hat{\rho}^{\frac{1}{2}} (\hat{x} - \langle \hat{x} \rangle_{\hat{\rho}^e}) \hat{\rho}^e (\hat{x} - \langle \hat{x} \rangle_{\hat{\rho}^e}) \hat{\rho}^{\frac{1}{2}} \right\} \geq 0, \tag{4.28}
\end{aligned}$$

which is what we had to show in order prove that the estimated state converges to the real one.

4.5 Remark

Continuous, unsharp, measurement of the state of a quantum system does not violate the rules of quantum mechanics. Given an individual quantum system whose state is unknown, one cannot deduce it by continuous observation because observing the state continuously drives it into a different one. Nevertheless, the continuous measurement with state-estimation scheme presented in this thesis enables one to prepare quantum states, monitor and control them.

Chapter 5

Numerical Simulation

5.1 Introduction

In this chapter we present the method to numerically simulate the monitoring of the position of a hydrogen atom, which is subject to several potentials. This constitutes to performing the experiment on a computer. For computational simplicity, we simulated the evolution of the stochastic wave function rather than the density matrix of the system. While there are several methods to numerically integrate stochastic differential equations, we shall only discuss a few: which include the Euler scheme and the second order weak scheme [30, 10, 47], which was suggested by Platen. The other methods can be found in [30, 10, 49, 31, 22, 40, 47]. Our stochastic differential equations are of the form,

$$d\psi(x, t) = a(\psi(x, t))dt + b(\psi(x, t))dW_t, \quad (5.1)$$

(see equations (3.53) and (4.17)) where $\psi(x, t) = \langle x | \psi(t) \rangle$ is the wave function of the system at a time t , $a(\psi(x, t))$ is a slowly varying function called the drift term, $b(\psi(x, t))$ is a rapidly fluctuating function called the diffusion term and dW_t is an infinitesimal increment of the Wiener process W at a time t . A way to derive the numerical integration scheme for equation (5.1), is to perform the Itô-Taylor expansion of the equation to a certain order and then deduce a discrete scheme. The theory of Itô-Taylor expansions is covered comprehensively in [30, 47, 49]. Here we shall only give a summary of the technique. To simplify the calculations we shall use ψ_t to represent $\psi(x, t)$. The integral version of the differential equation (5.1) is therefore given by:

$$\psi_t = \psi_{t_0} + \int_{t_0}^t a(\psi_s) ds + \int_{t_0}^t b(\psi_s) dW_s. \quad (5.2)$$

The simplest iterative scheme, the Euler scheme, can be derived by directly discretizing equation (5.1) in the manner that we will explain below. To solve the equation in the time interval $[0, T]$, we divide the interval into N equal partitions such that each partition is of the size $\Delta t = T/N$. We

thus define a discretization $\Delta_\tau := \{t_k : k = 0, 1, \dots, N : t_0 < t_1 < \dots < t_N = T\}$. Equation (5.1) can therefore be solved using the following discrete iterative formula:

$$\psi_{k+1} = \psi_k + a(\psi_k)\Delta t + b(\psi_k)\Delta W_k, \quad (5.3)$$

where k runs from 0 to $n - 1$, $\Delta W_k = W_{t_{k+1}} - W_{t_k}$ and $\psi_{k_0} = \psi_0$ an initial guess of the solution. Equation (5.3) is called the Euler scheme and converges with strong order 0.5. A discrete time approximation $\tilde{\psi}$, constructed on the time discretization Δ_τ , is said to converge with strong order p at a time t to the solution ψ of the stochastic differential equation (5.1) if there exist a constant C , which does not depend on Δt , such that

$$\langle |\psi_t - \tilde{\psi}_t| \rangle \leq C\Delta t^p. \quad (5.4)$$

On the other hand a discrete time approximation $\tilde{\psi}$, constructed on the time discretization Δ_τ , is said to converge with weak order p at a time t to the solution ψ of the stochastic differential equation (5.1) if for each function g there exist a constant C , which does not depend on Δt , such that

$$\langle |g(\psi_t) - g(\tilde{\psi}_t)| \rangle \leq C\Delta t^p, \quad (5.5)$$

see [49, 47]. The random variables ΔW_k are independent and normally distributed with expectation value 0 and variance Δt . One way to generate ΔW_k in a computer simulation is to use $\Delta W_k = \xi_k \sqrt{\Delta t}$, where ξ_k are standard normally distributed random variables that are generated using the Box-Muller method [9]. A C programming language library to implement the Box-Muller method can be found in [50]. A modified version of the Euler scheme, which has a strong convergence of order 1 was proposed by Milstein [39]. We will encounter it later. Firstly we shall go through the theory of Itô-Taylor expansions.

5.2 Itô-Taylor expansions

Itô-Taylor expansions are the stochastic analogy of deterministic Taylor expansions. In fact, the deterministic Taylor expansion is more often the convenient starting point in deriving the stochastic counterpart. Let us consider the following differential equation:

$$\frac{d}{dt}X_t = a(X_t), \quad (5.6)$$

with initial value X_{t_0} for $t \in [t_0, T]$. The differential equation (5.6) can be written symbolically in the following way:

$$dX_t = a(X_t) dt, \quad (5.7)$$

and more precisely represented by the following integral equation:

$$X_t = X_{t_0} + \int_{t_0}^t a(X_s) ds. \quad (5.8)$$

If a satisfies the Lipschitz condition:

$$|a(x) - a(y)| \leq C|x - y|, \quad (5.9)$$

as well as the linear growth bound condition:

$$|a(x)| \leq C(1 + |x|), \quad (5.10)$$

where $C > 0$ is some constant (see [51, 47]), then for any function f of X_t ,

$$\begin{aligned} \frac{d}{dt}f(X_t) &= \frac{dx}{dt} \frac{\partial}{\partial x} [f(X_t)] \\ &= a(X_t) \frac{\partial}{\partial x} [f(X_t)]. \end{aligned} \quad (5.11)$$

From equation (5.11) we define an operator $a\partial/\partial x$ as follows:

$$a \frac{\partial}{\partial x} f(X_t) := a(X_t) \frac{\partial}{\partial x} f(X_t). \quad (5.12)$$

The integral version of equation (5.11) can be written as follows:

$$f(X_t) = f(X_{t_0}) + \int_{t_0}^t a \frac{\partial}{\partial x} [f(X_s)] ds. \quad (5.13)$$

If $f(x) = x$, then $(a\partial/\partial x)f = a(X_s)$ and $(a\partial/\partial x)^2 f = (a\partial/\partial x)[a(X_s)]$. Thus we obtain equation (5.8) from (5.13). We now apply relation (5.13) to the function $f = a(X_s)$ in (5.8) to obtain

$$\begin{aligned} X_t &= X_{t_0} + \int_{t_0}^t \left[a(X_{t_0}) + \int_{t_0}^s a \frac{\partial}{\partial x} [a(X_u)] du \right] ds \\ &= X_{t_0} + \int_{t_0}^t a(X_{t_0}) ds + \int_{t_0}^t \int_{t_0}^s a \frac{\partial}{\partial x} [a(X_u)] du ds \\ &= X_{t_0} + a(X_{t_0}) \int_{t_0}^t ds + \int_{t_0}^t \int_{t_0}^s a \frac{\partial}{\partial x} [a(X_u)] du ds. \end{aligned} \quad (5.14)$$

If we apply the relation (5.13) to $f = (a\partial/\partial x)[a(X_u)]$ in (5.14), we obtain the following integral equation:

$$a \frac{\partial}{\partial x} a(X_u) = a \frac{\partial}{\partial x} \left[a(X_{t_0}) + \int_{t_0}^u a \frac{\partial}{\partial x} [a(X_v)] dv \right]. \quad (5.15)$$

We now substitute equation (5.15) into (5.14) to obtain

$$\begin{aligned}
X_t &= X_{t_0} + a(X_{t_0}) \int_{t_0}^t ds + \int_{t_0}^t \int_{t_0}^s a \frac{\partial}{\partial x} \left[a(X_{t_0}) + \int_{t_0}^u a \frac{\partial}{\partial x} [a(X_v)] dv \right] du ds \\
&= X_{t_0} + a(X_{t_0}) \int_{t_0}^t ds + \int_{t_0}^t \int_{t_0}^s a \frac{\partial}{\partial x} [a(X_{t_0})] du ds + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u a^2 \frac{\partial^2}{\partial x^2} [a(X_v)] dv du ds \\
&= X_{t_0} + a(X_{t_0}) \int_{t_0}^t ds + a \frac{\partial}{\partial x} [a(X_{t_0})] \int_{t_0}^t \int_{t_0}^s du ds + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u a^2 \frac{\partial^2}{\partial x^2} [a(X_v)] dv du ds.
\end{aligned} \tag{5.16}$$

We can continue the scheme apply relation (5.13) to $(a\partial/\partial x)^2[a(X_v)]$ the same way as we have done to $f = (a\partial/\partial x)[a(X_u)]$ and $f = a(X_s)$ for as long as $a(X_v)$ is smooth and differentiable. However, from comparing equations (5.8), (5.14) and (5.16) we can clearly see a pattern, which we will generalize below as follows:

$$\begin{aligned}
X_t &= X_{t_0} + a(X_{t_0}) \int_{t_0}^t ds_1 + a \frac{\partial}{\partial x} [a(X_{t_0})] \int_{t_0}^t \int_{t_0}^{s_1} ds_2 ds_1 \\
&\quad + a^2 \frac{\partial^2}{\partial x^2} [a(X_{t_0})] \int_{t_0}^t \int_{t_0}^{s_1} \int_{t_0}^{s_2} ds_3 ds_2 ds_1 \\
&\quad + a^{n-1} \frac{\partial^{n-1}}{\partial x^{n-1}} [a(X_{t_0})] \int_{t_0}^t \dots \int_{t_0}^{s_{n-1}} ds_n \dots ds_1 \\
&\quad + \int_{t_0}^t \dots \int_{t_0}^{s_n} a^n \frac{\partial^n}{\partial x^n} [a(X_{s_{n+1}})] ds_{s_{n+1}} \dots ds_1.
\end{aligned} \tag{5.17}$$

We can explicitly evaluate all of the integrals, except the last, in equation (5.17). The single integral evaluates to $t - t_0$ and the multiple integrals are evaluated using the following formula:

$$\int_{t_0}^t \dots \int_{t_0}^{s_m} ds_{m+1} \dots ds_1 = \frac{1}{(m+1)!} (t - t_0)^{m+1}, \tag{5.18}$$

for $m = 1, 2, \dots, n - 1$. Substituting equation (5.18) into equation (5.17), we obtain

$$X_t = X_{t_0} + \sum_{m=0}^{n-1} \frac{(t-t_0)^{m+1}}{(m+1)!} a^m \frac{\partial^m}{\partial x^m} [a(X_{t_0})] + \int_{t_0}^t \dots \int_{t_0}^{s_n} a^n \frac{\partial^n}{\partial x^n} [a(X_{s_{n+1}})] ds_{s_{n+1}} \dots ds_1. \quad (5.19)$$

Equation (5.19) is the Taylor expansion in t of equation (5.8). From equation (5.19) we can derive iterative schemes of desired order of convergence to solve equation (5.6) by setting $t - t_0 = \Delta t$ and ignoring the multiple integral term. For example, if $n = 1$ one obtains the deterministic Euler scheme. Now that we have the general idea on how to Taylor-expand ordinary differential equations, we are in a position to attempt the same for stochastic differential equations of the form

$$dX_t = a(X_t) dt + b(X_t) dW_t. \quad (5.20)$$

Equation (5.20) can be written precisely in the following way:

$$X_t = X_{t_0} + \int_{t_0}^t a(X_s) ds + \int_{t_0}^t b(X_s) dW_s. \quad (5.21)$$

According to Itô's lemma [28], a function f of a stochastic variable X_t that evolves according to equation (5.20) is given by:

$$\begin{aligned} f(X_t) = & f(X_{t_0}) + \int_{t_0}^t \left[a(X_s) \frac{\partial}{\partial x} f(X_s) + \frac{1}{2} b^2(X_s) \frac{\partial^2}{\partial x^2} f(X_s) \right] ds \\ & + \int_{t_0}^t b(X_s) \frac{\partial}{\partial x} f(X_s) dW_s. \end{aligned} \quad (5.22)$$

The last integral terms in equations (5.21) and (5.22) are called Itô integrals and cannot be treated as Riemann integrals. The technique to evaluate them is covered extensively in [47, 30, 49]. Taking a similar approach as in the deterministic case we define operators

$$L_0 = a \frac{\partial}{\partial x} + \frac{1}{2} b^2 \frac{\partial^2}{\partial x^2} \quad (5.23)$$

and

$$L_1 = b \frac{\partial}{\partial x} \quad (5.24)$$

as follows:

$$L_0 X_t := a(X_t) \frac{\partial}{\partial x} f(X_t) + \frac{1}{2} b^2(X_t) \frac{\partial^2}{\partial x^2} f(X_t) \quad (5.25)$$

and

$$L_1 X_t := b(X_t) \frac{\partial}{\partial x} f(X_t). \quad (5.26)$$

For $f(x) = x$ equation (5.22) reduces to equation (5.21). Applying relation (5.22) to $f = a(X_s)$ and $f = b(X_s)$ in equation (5.21), we obtain

$$\begin{aligned} X_t &= X_{t_0} \\ &+ \int_{t_0}^t \left(a(X_{t_0}) + \int_{t_0}^s L_0 a(X_u) du + \int_{t_0}^s L_1 a(X_u) dW_u \right) ds \\ &+ \int_{t_0}^t \left(b(X_{t_0}) + \int_{t_0}^s L_0 b(X_u) du + \int_{t_0}^s L_1 b(X_u) dW_u \right) dW_s \\ &= X_{t_0} + a(X_{t_0}) \int_{t_0}^t ds + b(X_{t_0}) \int_{t_0}^t dW_s \\ &+ \int_{t_0}^t \int_{t_0}^s L_0 a(X_u) du ds + \int_{t_0}^t \int_{t_0}^s L_1 a(X_u) dW_u ds \\ &+ \int_{t_0}^t \int_{t_0}^s L_0 b(X_u) du dW_s + \int_{t_0}^t \int_{t_0}^s L_1 b(X_u) dW_u dW_s. \end{aligned} \quad (5.27)$$

If we apply the relation (5.22) to $f = L_0 a(X_u)$, $f = L_1 a(X_u)$, $f = L_0 b(X_u)$, and $f = L_1 b(X_u)$ in (5.27) we get the following:

$$L_0 a(X_u) = L_0 a(X_{t_0}) + \int_{t_0}^u L_0^2 a(X_v) dv + \int_{t_0}^u L_1 L_0 a(X_v) dW_v, \quad (5.28)$$

$$L_1 a(X_u) = L_1 a(X_{t_0}) + \int_{t_0}^u L_0 L_1 a(X_v) dv + \int_{t_0}^u L_1^2 a(X_v) dW_v, \quad (5.29)$$

$$L_0 b(X_u) = L_0 b(X_{t_0}) + \int_{t_0}^u L_0^2 b(X_v) dv + \int_{t_0}^u L_1 L_0 b(X_v) dW_v, \quad (5.30)$$

$$L_1 b(X_u) = L_1 b(X_{t_0}) + \int_{t_0}^u L_0 L_1 b(X_v) dv + \int_{t_0}^u L_1^2 b(X_v) dW_v. \quad (5.31)$$

Substituting equations (5.28), (5.29), (5.30) and (5.31) into (5.27), we obtain the following:

$$\begin{aligned}
X_t = & X_{t_0} + a(X_{t_0}) \int_{t_0}^t ds + b(X_{t_0}) \int_{t_0}^t dW_s \\
& + L_0 a(X_{t_0}) \int_{t_0}^t \int_{t_0}^s du ds + L_1 a(X_{t_0}) \int_{t_0}^t \int_{t_0}^s dW_u ds \\
& + L_0 b(X_{t_0}) \int_{t_0}^t \int_{t_0}^s du dW_s + L_1 b(X_{t_0}) \int_{t_0}^t \int_{t_0}^s dW_u dW_s \\
& + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_0^2 a(X_v) dv du ds + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_1 L_0 a(X_v) dW_v du ds \\
& + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_0 L_1 a(X_v) dv dW_u ds + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_1^2 a(X_v) dW_v dW_u ds \\
& + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_0^2 b(X_v) dv du dW_s + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_1 L_0 b(X_v) dW_v du dW_s \\
& + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_0 L_1 b(X_v) dv dW_u dW_s + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_1^2 b(X_v) dW_v dW_u dW_s. \tag{5.32}
\end{aligned}$$

We can re-write equation (5.32) in the following way,

$$X_t = X_{t_0} + a(X_{t_0}) \int_{t_0}^t ds + b(X_{t_0}) \int_{t_0}^t dW_s + L_1 b(X_{t_0}) \int_{t_0}^t \int_{t_0}^s dW_u dW_s + R, \tag{5.33}$$

where

$$\begin{aligned}
R = & L_0 a(X_{t_0}) \int_{t_0}^t \int_{t_0}^s du ds + L_1 a(X_{t_0}) \int_{t_0}^t \int_{t_0}^s dW_u ds + L_0 b(X_{t_0}) \int_{t_0}^t \int_{t_0}^s du dW_s \\
& + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_0^2 a(X_v) dv du ds + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_1 L_0 a(X_v) dW_v du ds \\
& + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_0 L_1 a(X_v) dv dW_u ds + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_1^2 a(X_v) dW_v dW_u ds \\
& + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_0^2 b(X_v) dv du dW_s + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_1 L_0 b(X_v) dW_v du dW_s \\
& + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_0 L_1 b(X_v) dv dW_u dW_s + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_1^2 b(X_v) dW_v dW_u dW_s. \tag{5.34}
\end{aligned}$$

Next we evaluate the integrals in (5.33) as follows:

$$\int_{t_0}^t ds = t - t_0, \tag{5.35}$$

$$\int_{t_0}^t dW_s = W_t - W_{t_0}, \tag{5.36}$$

and

$$\int_{t_0}^t \int_{t_0}^s dW_u dW_s = \frac{1}{2} [(W_t - W_{t_0})^2 - (t - t_0)]. \tag{5.37}$$

Substituting equations (5.35), (5.36) and (5.37) into (5.33), we obtain

$$\begin{aligned}
X_t = & X_{t_0} + a(X_{t_0})[t - t_0] + b(X_{t_0})[W_t - W_{t_0}] \\
& + \frac{1}{2} b(X_{t_0}) \frac{\partial}{\partial x} b(X_{t_0}) [(W_t - W_{t_0})^2 - (t - t_0)] + R, \tag{5.38}
\end{aligned}$$

If we replace our stochastic variable X_t with ψ_t and apply the discretization Δ_τ to equation (5.38) as we did to equation (5.1) we obtain the following iterative formula:

$$\begin{aligned}\psi_{k+1} = & \psi_k + a(\psi_k)\Delta t + b(\psi_k)\Delta W_k \\ & + \frac{1}{2}b(\psi_k)\frac{\partial}{\partial x}b(\psi_k)\left[\Delta W_k^2 - \Delta t\right],\end{aligned}\tag{5.39}$$

by setting $t - t_0 = \Delta t$, $W_t - W_{t_0} = \Delta W_t$ and truncating the remainder. Equation (5.39) is the Milstein scheme [39].

5.3 Second order weak scheme

In this section we give a summary on how to derive the second order weak scheme, which we used to numerically simulate the monitoring of the wave function of the hydrogen atom that is subjected to several potentials. The second order weak scheme was suggested by Platen [30, 10, 47] and has also been used in [53]. In order for us to derive the scheme we start with equation (5.32) written in the following way:

$$\begin{aligned}X_t = & X_{t_0} + a(X_{t_0}) \int_{t_0}^t ds + b(X_{t_0}) \int_{t_0}^t dW_s \\ & + L_0 a(X_{t_0}) \int_{t_0}^t \int_{t_0}^s du ds + L_1 a(X_{t_0}) \int_{t_0}^t \int_{t_0}^s dW_u ds \\ & + L_0 b(X_{t_0}) \int_{t_0}^t \int_{t_0}^s du dW_s + L_1 b(X_{t_0}) \int_{t_0}^t \int_{t_0}^s dW_u dW_s + R,\end{aligned}\tag{5.40}$$

where

$$\begin{aligned}
R = & \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_0^2 a(X_v) dv du ds + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_1 L_0 a(X_v) dW_v du ds \\
& + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_0 L_1 a(X_v) dv dW_u ds + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_1^2 a(X_v) dW_v dW_u ds \\
& + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_0^2 b(X_v) dv du dW_s + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_1 L_0 b(X_v) dW_v du dW_s \\
& + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_0 L_1 b(X_v) dv dW_u dW_s + \int_{t_0}^t \int_{t_0}^s \int_{t_0}^u L_1^2 b(X_v) dW_v dW_u dW_s. \tag{5.41}
\end{aligned}$$

We then evaluate the integrals in equation (5.40), using the scheme given in [30, 47] as follows:

$$\int_{t_0}^t ds = t - t_0, \tag{5.42}$$

$$\int_{t_0}^t dW_s = W_t - W_{t_0}, \tag{5.43}$$

$$\int_{t_0}^t \int_{t_0}^s du ds = \frac{1}{2}(t - t_0)^2, \tag{5.44}$$

$$\int_{t_0}^t \int_{t_0}^s dW_u dW_s = \frac{1}{2}[(W_t - W_{t_0})^2 - (t - t_0)], \tag{5.45}$$

$$\int_{t_0}^t \int_{t_0}^s dW_u ds := \Delta Z, \tag{5.46}$$

and

$$\int_{t_0}^t \int_{t_0}^s du dW_s = (W_t - W_{t_0})(t - t_0) - \Delta Z, \tag{5.47}$$

where ΔZ is Gaussian distributed with mean $\langle \Delta Z \rangle = 0$, variance $\langle \Delta Z^2 \rangle = \frac{1}{3} \Delta t^3$ and covariance $\langle \Delta Z \Delta W \rangle = \frac{1}{2} \Delta t^2$. In a numerical simulation one can generate ΔW and ΔZ using the following formulas:

$$\Delta W = \xi_1 \sqrt{\Delta t} \quad (5.48)$$

and

$$\Delta Z = \frac{1}{2} \left(\xi_1 + \frac{1}{\sqrt{3}} \xi_2 \right) \Delta t^{\frac{3}{2}}, \quad (5.49)$$

where ξ_1 and ξ_2 are independent standard Gaussian distributed random variables. Substituting equations (5.42) through to (5.47) into (5.40), we obtain

$$\begin{aligned} X_t = & X_{t_0} + a(X_{t_0})(t - t_0) + b(X_{t_0})(W_t - W_{t_0}) \\ & + \frac{1}{2} L_0 a(X_{t_0})(t - t_0)^2 + L_1 a(X_{t_0}) \Delta Z \\ & + L_0 b(X_{t_0})[(W_t - W_{t_0})(t - t_0) - \Delta Z] \\ & + \frac{1}{2} L_1 b(X_{t_0})[(W_t - W_{t_0})^2 - (t - t_0)] + R. \end{aligned} \quad (5.50)$$

If we replace our stochastic variable X_t with ψ_t and apply the discretization Δ_τ to equation (5.51), we obtain the following iterative formula:

$$\begin{aligned} \psi_{k+1} = & \psi_k + a(\psi_k) \Delta t + b(\psi_k) \Delta W \\ & + \frac{1}{2} L_0 a(\psi_k) \Delta t^2 + L_1 a(\psi_k) \Delta Z \\ & + L_0 b(\psi_k) [\Delta W \Delta t - \Delta Z] \\ & + \frac{1}{2} L_1 b(\psi_k) [\Delta W^2 - \Delta t], \end{aligned} \quad (5.51)$$

after truncating the remainder and setting $t - t_0 = \Delta t$. Equation (5.51) is the second order weak Taylor scheme that was given in [30]. If we go on and replace the derivatives in L_0 and L_1 with finite differences, we obtain the following scheme, which was given by Platen [30, 10]:

$$\begin{aligned} \psi_{k+1} = & \psi_k \\ & + \frac{1}{2} \left(a(\psi_k) + a(\tilde{\psi}_k) \right) \Delta t \\ & + \frac{1}{4} \left(b(\psi_k^+) + b(\psi_k^-) + 2b(\psi_k) \right) \Delta W_k \\ & + \frac{1}{4} \left(b(\psi_k^+) - b(\psi_k^-) \right) \left(\Delta W_k^2 - \Delta t \right) \sqrt{\Delta t}, \end{aligned} \quad (5.52)$$

with

$$\tilde{\psi}_k = \psi_k + a(\psi_k) \Delta t + b(\psi_k) \Delta W_k \quad (5.53)$$

and

$$\psi_k^\pm = \psi_k + a(\psi_k)\Delta t \pm b(\psi_k)\sqrt{\Delta t}. \quad (5.54)$$

Given the stochastic Schrödinger equations (3.53) and (4.17) for the true wave function ψ and estimated wave function ψ^e in one spatial dimension x , the terms a and b are given by the following:

$$a(\psi_k) = \left(-\frac{i}{\hbar}\hat{H} - \frac{\gamma}{8}(\hat{x} - \langle \hat{x} \rangle_{\psi_k})^2 \right) \psi_k, \quad (5.55)$$

$$b(\psi_k) = \frac{\gamma}{2}(\hat{x} - \langle \hat{x} \rangle_{\psi_k})\psi_k, \quad (5.56)$$

$$a(\psi_k^e) = \left(-\frac{i}{\hbar}\hat{H} - \frac{\gamma}{8}(\hat{x} - \langle \hat{x} \rangle_{\psi_k^e})^2 + \frac{\gamma}{2}(\hat{x} - \langle \hat{x} \rangle_{\psi_k^e})(\langle \hat{x} \rangle_{\psi_k} - \langle \hat{x} \rangle_{\psi_k^e}) \right) \psi_k^e \quad (5.57)$$

and

$$b(\psi_k^e) = \frac{\gamma}{2}(\hat{x} - \langle \hat{x} \rangle_{\psi_k^e})\psi_k^e, \quad (5.58)$$

where \hat{H} is the Hamiltonian of the system given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x), \quad (5.59)$$

p is the momentum of the hydrogen atom, $m = m_e + m_p$ is the rest mass of the hydrogen atom, m_e is the rest mass of electron, m_p is the mass of proton and $V(x)$ is the potential energy at a point x . The numerical simulations are performed in the non-relativistic frame. The initial true wave function $\psi(x, t_0)$ is given by the following function:

$$\psi(x) = \frac{1}{\sqrt[4]{2\pi\sigma_x^2}} \exp\left(-ikx\right) \exp\left(\frac{-(x - \bar{x})^2}{4\sigma_x^2}\right), \quad (5.60)$$

where $k = p/\hbar$ is the wave number, \bar{x} is the expectation value of x and σ_x is the standard deviation of x . Wave functions of the form of $\psi(x)$ are referred to as Gaussian because they generate normal probability distributions,

$$\varrho(x) = \psi(x)^* \psi(x) = |\psi(x)|^2 = \frac{1}{\sqrt{2\pi\sigma_x^2}} \exp\left(\frac{-(x - \bar{x})^2}{2\sigma_x^2}\right). \quad (5.61)$$

So far we have only discretized time but in order for us to perform a numerical simulation in a computer we need to discretize space as well. We introduce a discretization $\Delta_x := \{x_j : j = 0, 1, \dots, M : x_0 = x_l < x_1 < \dots < x_M = x_r\}$ of the interval $[x_l, x_r]$ by dividing the interval into M equal partitions. The width of each partition is therefore given by $\Delta x = (x_r - x_l)/M$.

Our numerical scheme requires that we give the position representation of the momentum operator \hat{p} in the kinetic energy term of the Hamiltonian \hat{H} as well as evaluate the expectation value of \hat{x} . From quantum mechanics we know that

$$\hat{p} = -i\hbar\nabla = -i\hbar\frac{\partial}{\partial x} \quad (5.62)$$

in one spatial dimension. This implies that

$$\frac{\hat{p}^2}{2m}\psi = \lim_{\Delta x \rightarrow 0} \frac{\hbar^2}{2m} \left(\frac{\psi_{j+1} + \psi_{j-1} - 2\psi_j}{\Delta x^2} \right). \quad (5.63)$$

The expectation value of \hat{x} is evaluated as follows:

$$\langle \hat{x} \rangle_\psi = \int_{-\infty}^{\infty} x \psi^* \psi \, dx = \lim_{M \rightarrow +\infty} \sum_{j=0}^M x_j \psi_j^* \psi_j \Delta x. \quad (5.64)$$

The variance of x , which we denote by Δx^2 is therefore given by

$$\begin{aligned} \Delta x^2 &= \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2 = \int_{-\infty}^{\infty} x^2 \psi^* \psi \, dx - \left(\int_{-\infty}^{\infty} x \psi^* \psi \, dx \right)^2 \\ &= \lim_{M \rightarrow +\infty} \sum_{j=0}^M x_j^2 \psi_j^* \psi_j \Delta x - \left(\lim_{M \rightarrow +\infty} \sum_{j=0}^M x_j \psi_j^* \psi_j \Delta x \right)^2. \end{aligned} \quad (5.65)$$

Equation (5.60) through to (5.65) also apply to the estimated wave function.

5.4 Numerical Results

The continuous measurement and estimation of the position of a hydrogen atom was numerically simulated using the second order weak scheme, which we described earlier. The simulations were limited to one-dimensional wave functions, due to limitations in computational power. Nevertheless, we managed to simulate the dynamics of the real and estimated wave functions of a free hydrogen atom, as well as an atom bounded in the potentials: harmonic

$$V(x) = \frac{1}{2} m \omega^2 x^2, \quad (5.66)$$

and double well,

$$V(x) = -\frac{8E}{w^2} x^2 + \frac{16E}{w^4} x^4, \quad (5.67)$$

where m is the rest mass of the hydrogen atom, ω is angular frequency, x is position, w is the distance from minima to minima in the double well potential, and E is the energy gap between minima and maxima (see figure 5.2). This was the first time the dynamics of the state of a quantum particle undergoing continuous measurement in the harmonic potential was investigated. The harmonic potential is shown in figure 5.1. The important point which we intended to show through the numeric

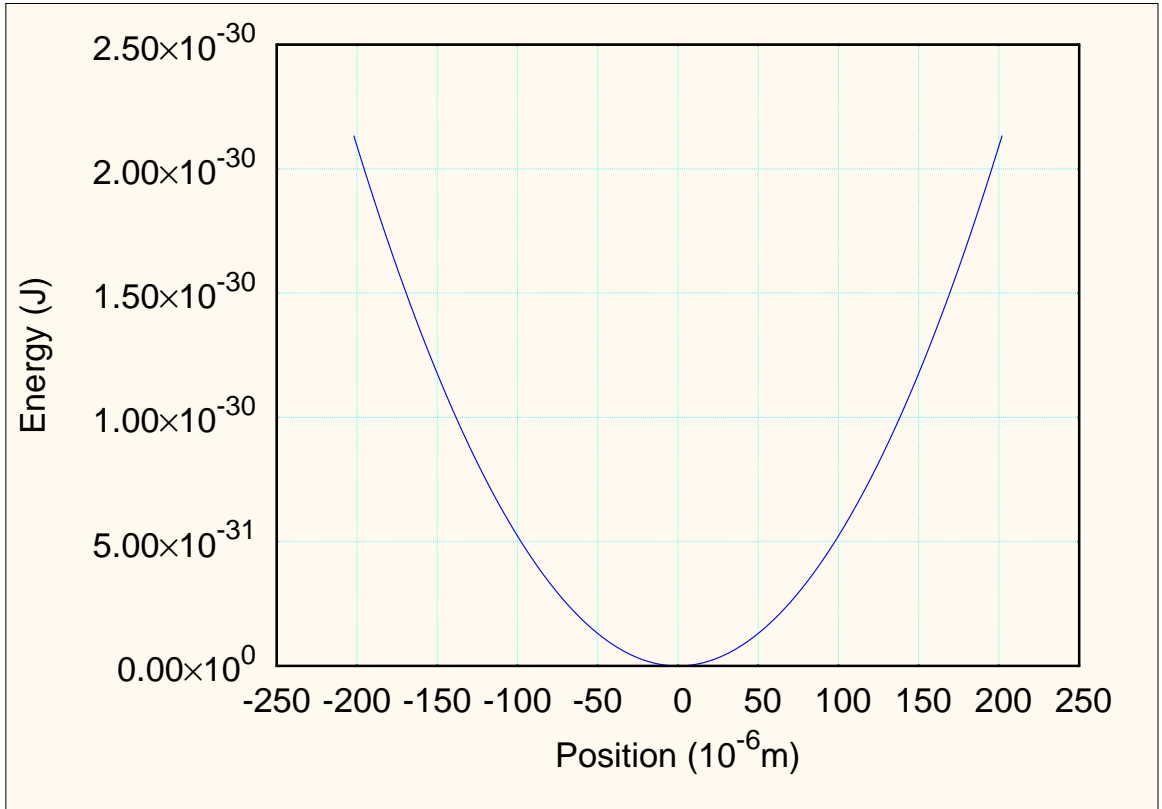


Figure 5.1: Harmonic potential.

simulations is that the weak measurement and state estimation scheme is suitable for monitoring the position of a single quantum system, in our case hydrogen atom, in real time irregardless of the potential in which the system is bound. This means that we were interested more in the convergence of the estimated state to the real one.

For the simulations that involved single runs we set our initial parameters as follows:

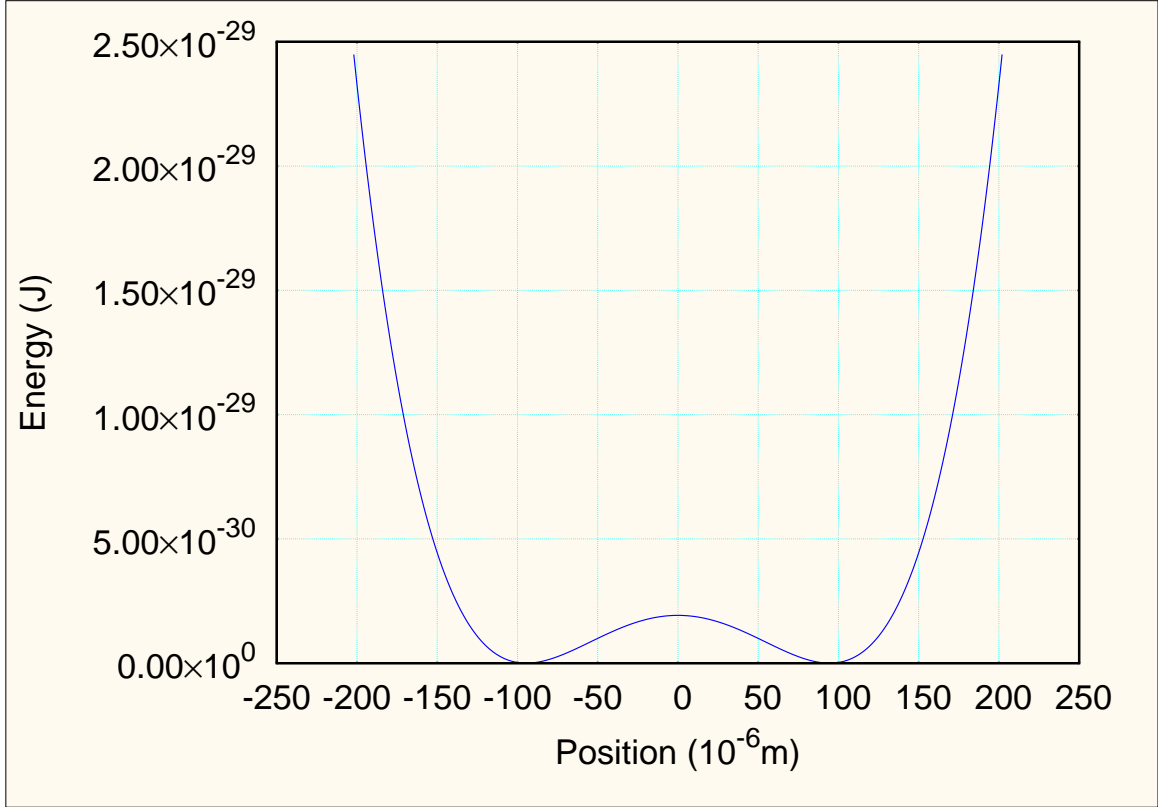


Figure 5.2: Double well potential.

- width of the real wave function $\delta = 10 \mu m$,
- width of the estimated wave function $\delta_e = 5 \mu m$,
- position of the centre of the real wave packet $x_0 = 0 m$ relative to the chosen centre of the simulated region,
- position of the centre of the estimated wave packet $x_{0_e} = +50 m$ relative to the chosen centre of the simulated region,
- the wave number $k = 0 m^{-1}$,
- angular frequency $\omega = 250 rad.s^{-1}$,
- distance between the two minimas in the double well potential $w = 189 \mu m$,

- energy difference between minima and maxima energies of the double well potential $E = 1.2 \times 10^{-11} \text{ eV}$,
- measurement strength $\gamma = 1 \times 10^{13} \text{ m}^{-2}\text{s}$,
- spatial resolution $\Delta x = 1 \text{ }\mu\text{m}$,
- temporal resolution $\Delta t = 100 \text{ ns}$,
- simulated region in space $R = [-200, 200] \text{ }\mu\text{m}$, where we chose the zero point to be the centre of the region.

5.4.1 Preliminary

Before performing any numerical simulations we tested the random number generator to verify if it could generate normally-distributed random number sets of the required size, which in our case was 900000. We also verified if each set would be independent of each other. We had to perform these tests because we did not devise the program implementation of the random number generator on our own, but rather borrowed it from Numerical Recipes [50]. The result of the former test is shown in figure 5.3 and the result of the latter test is shown in figure 5.4. To obtain figure 5.3, we generated a set of 900000 random numbers, determined the relative frequency of its subsets, which we obtained by dividing the interval $[-10, 10]$ into smaller intervals of width 0.01, and then plotted the distribution of the relative frequency. The red line represents the distribution of the relative frequency whilst the black line represents the normal probability distribution with mean 0 and variance 1. From figures 5.3 and 5.4 we can conclude that the random number generator was fit for use in our numerical simulations since the relative frequency curve reasonably approximates the standard normal distribution and each data set follows a different sample path.

5.4.2 Convergence

As suggested by the theory, the convergence of the estimated wave function to the real wave function was observed in all the three cases, which we investigated. If we look at figures 5.5 a) 5.6 a) and 5.7 a), we can see that the fidelity starts at 0, and in time it rises until it asymptotically reaches unity. This means that even if the estimated wave function and the true wave function do not overlap initially, given enough time, they fully overlap each other and the estimated wave function fully describes the state of the system.

The argument in the previous paragraph is further strengthened by the results shown in figures 5.8, 5.9 and 5.10. These results were obtained after running the simulations 1000 times with the same initial conditions, for each of the three cases, and determining the average fidelity and its standard deviation at specific times. Again we see that the average fidelity starts at 0 and then rises until it reaches unity. The average fidelity curve is smooth whereas the one for the single runs is wiggly.

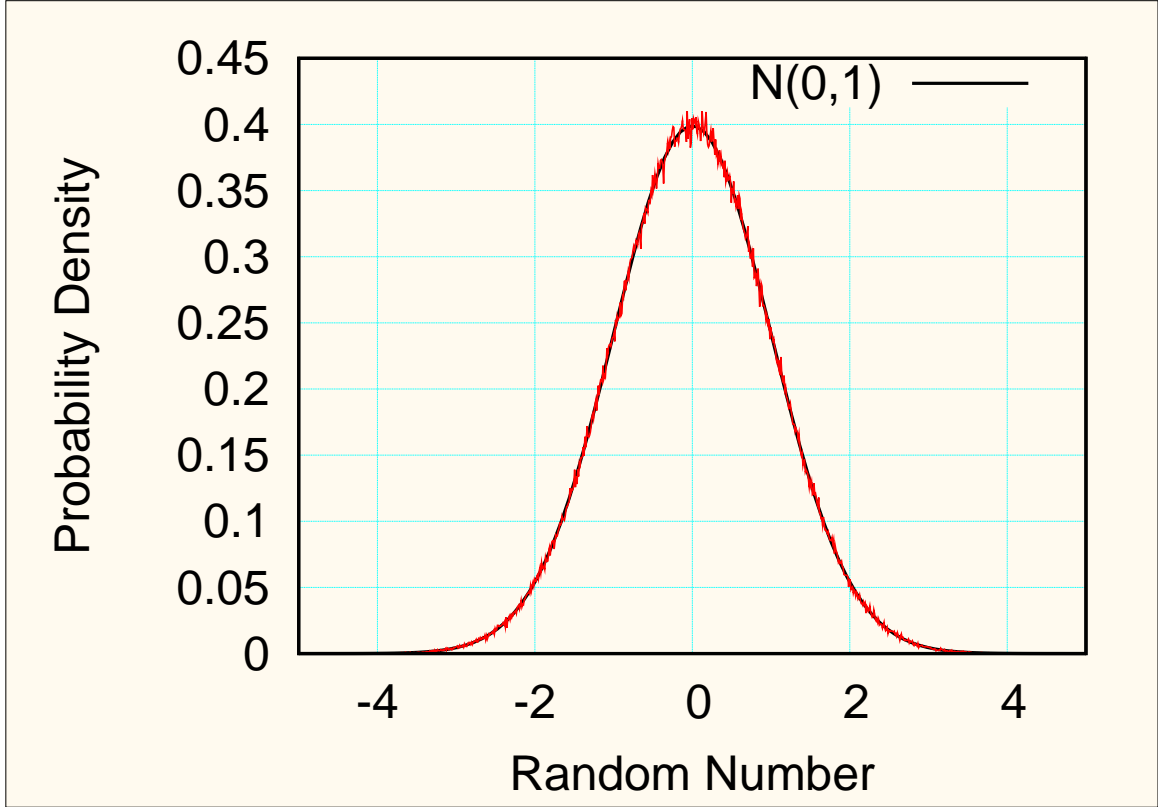


Figure 5.3: The comparison between the relative frequency of the generated random numbers (red) with the standard normal distribution (black). A sample of 900000 random numbers was generated.

The wiggly behaviour stems from the stochastic evolution of both the true and the estimated wave functions. The error bars in figures 5.8, 5.9 and 5.10 confirm that, indeed, fidelity is a stochastic variable for the cases that we investigated. This implies that, given the same initial conditions, the fidelity takes a different path for each of the runs.

For single runs, the convergence time of the wave functions for the free particle was found to be approximately $9ms$, whilst the convergence time for the hydrogen atom in the harmonic and double well potentials was found to be $8.5ms$ and $10ms$, respectively. The wave functions for the particle in the harmonic potential converge faster than in the case of the free particle or particle in the double well potential due to the fact that harmonic potential bounds the particle in a much smaller region in space as compared to the other two cases.

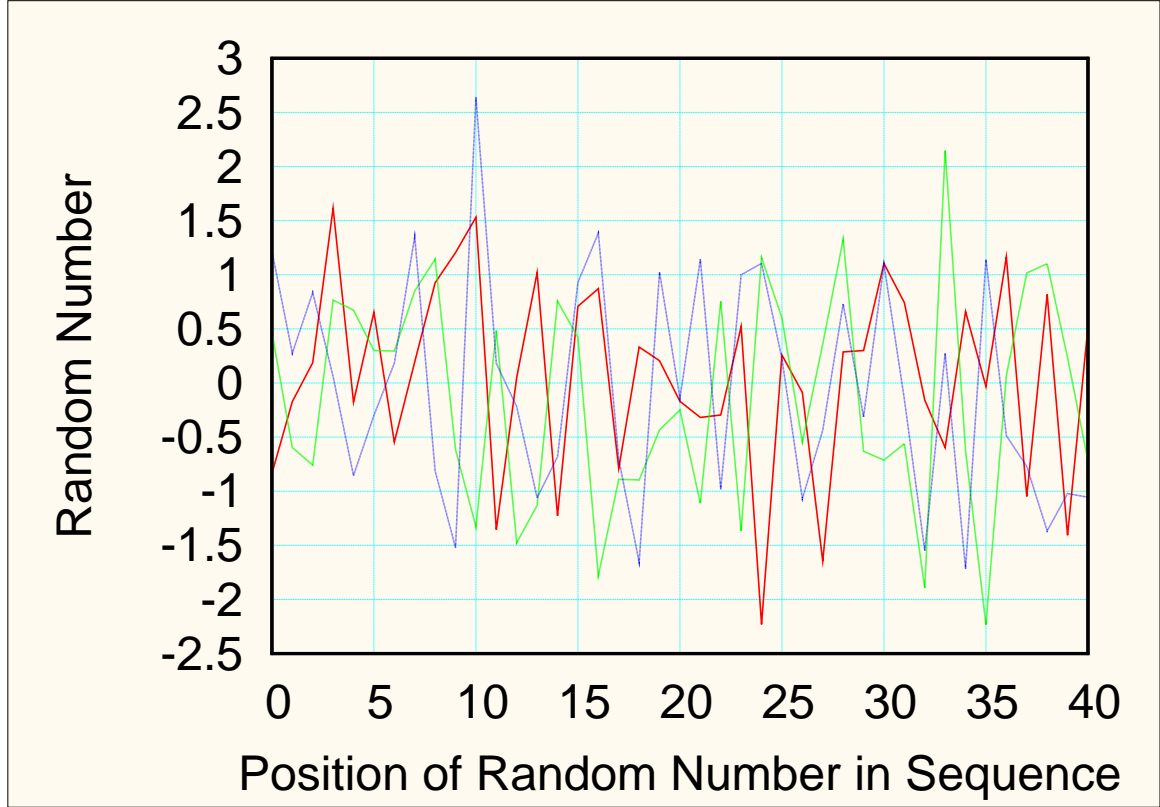


Figure 5.4: Sequences of the first forty random numbers generated on three test runs of the Gaussian random number generator.

5.4.3 Effects of continuous selective measurement

Figures 5.5 c) and d), 5.6 c) and d), and 5.7 c) and d) illustrate the effects of selective measurement. To explain the phenomena we first focus our attention on the free particle case. In the absence of measurement, the Gaussian wave function spreads indefinitely. Indeed the evolution equations (3.53) and (4.17) become normal Schrödinger equations, which are diffusive in nature. Selective measurement localizes the wave function (that is, it give the wave function a finite width) as shown in figure 5.5 d). We see that in the case of the free hydrogen atom, the standard deviation of the position (which is a measure of the width of the wave function) starts at the value we set initially ($10 \mu m$ and $5 \mu m$ for the true and estimated wave functions respectively) and then it decreases (in the case of the true wave function) and rises (in the case of the estimated wave function) until it reaches a value of about $9 \mu m$ and stays almost constant until a time of $0.05s$, where the wave

functions hit one of the boundaries of our domain of x -values for the first time causing the width to fall sharply. The wave functions also hit boundaries at times $0.065s$ and $0.08s$. The fall in the size of the width of the wave function at the boundaries is merely due to the fact that the boundaries are not mathematically well defined. This implies that if we had simulated a larger region in space the dips would not have occurred at those times. This is different, however, in the case where we have potentials where we expect the widths of the wave functions to fall each time the particle moves towards higher potentials. This is clearly illustrated in figure 5.7 d) for the case of the hydrogen atom in the double well potential. If we compare the position (given in figure 5.7 c)) with standard deviation of position (given in figure 5.7 d)), we can see that every time the particle moves towards a region with higher potential energy its width falls and each time it moves towards the centre of either potential wells the width increases. However, it is interesting to see that in the case where we bound our particle in the harmonic potential the wave functions seem to maintain a constant width (as indicated by a standard deviation of position of about $8.5 \mu m$), which they attain at time $0.01s$.

Selective measurement also makes the hydrogen atom take a random walk when it absorbs energy from the measuring device. Again it is easier to explain this phenomena using a free hydrogen atom. We already know that in the absence of measurement our wave functions diffuse. When this happens the centre of the wave packet does not move. Now in the case where we measure the position non-selectively, we get the localization of the wave packet but again the centre of the wave packet remains stationary. In case of selective measurement, the centre of the wave function moves each time a measurement is taken on the system. The motion is random and hence the term ‘random walk’ is used. The behaviour is illustrated by the wiggly and irregular nature of plots of the position of the hydrogen atom over time shown in figures 5.5 c), 5.6 c), and 5.7 c).

5.4.3.1 The variation of estimated convergence time with measurement strength γ

Konrad and Uys [33] applied the theory of continuous measurement and estimation to the problem monitoring the state of a two level system undergoing Rabi oscillations in the presence of various noises. They investigated the dependence of the convergence time on the measurement strengths. Clearly in the case where there was no classical noise (Fig. 4b of [33]) they obtained results suggesting some power law variation. We followed a similar approach, by keeping all the other free parameters constant and varying only the measurement strengths, and obtained similar results as shown in figures 5.11, 5.12 and 5.13. It is important to note that the results we present here are for single runs of the numerical simulations whilst Konrad and Uys plotted the average values of several runs. Our results are however quite encouraging, especially in the case of the free particle where we get reasonably linear variation. In order to approximate the convergence time, we took the numerical value of the asymptotic fidelity to be 0.999995 , which is reasonably close to 1. However, this value can be improved in future investigations in order to obtain a more accurate convergence time. By letting the convergence time be denoted by t_c we can derive the power law from the following

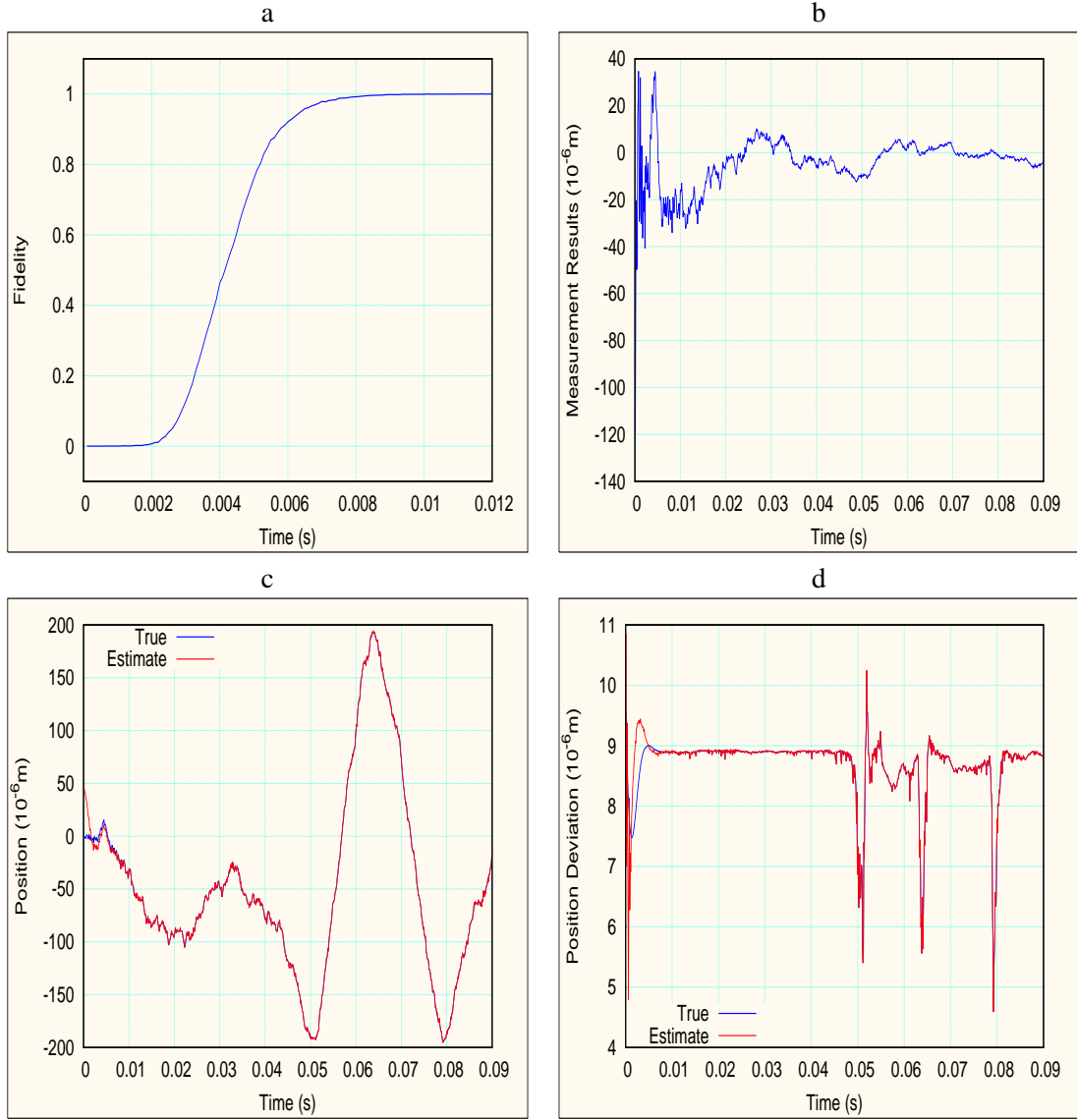


Figure 5.5: Results of the simulation of the evolution of the one dimensional wave function of a free hydrogen atom whose position is continuously monitored. a) The evolution of fidelity with time. b) The variation of averaged measurement results with time. c) The variation of the mean position of the atom with time. d) The variation of the deviation of position with time.

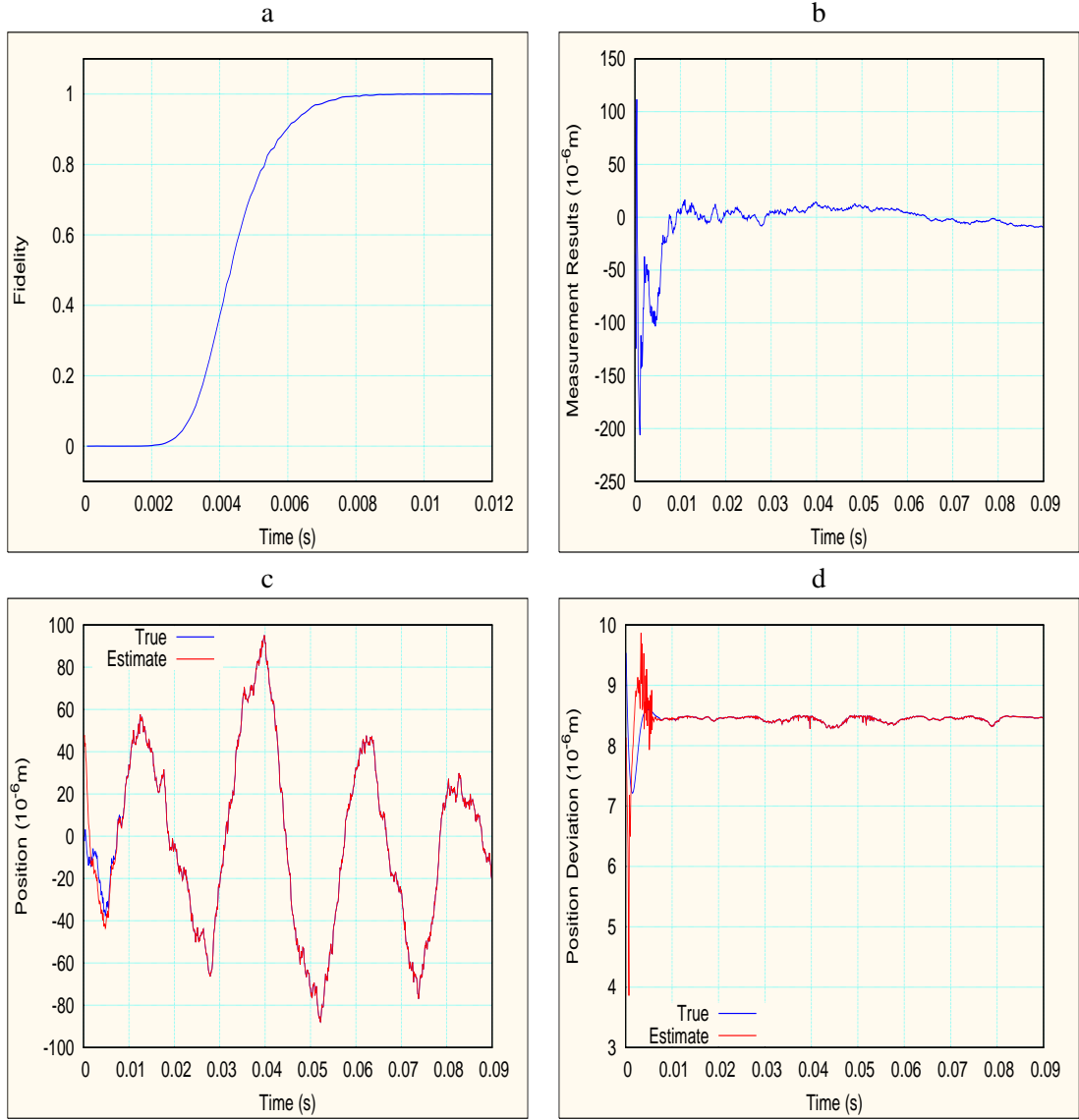


Figure 5.6: Results of the simulation of the evolution of the one dimensional wave function of a hydrogen atom in a harmonic potential whose position is continuously monitored. a) The evolution of fidelity with time. b) The variation of averaged measurement results with time. c) The variation of the mean position of the atom with time. d) The variation of the deviation of position with time.

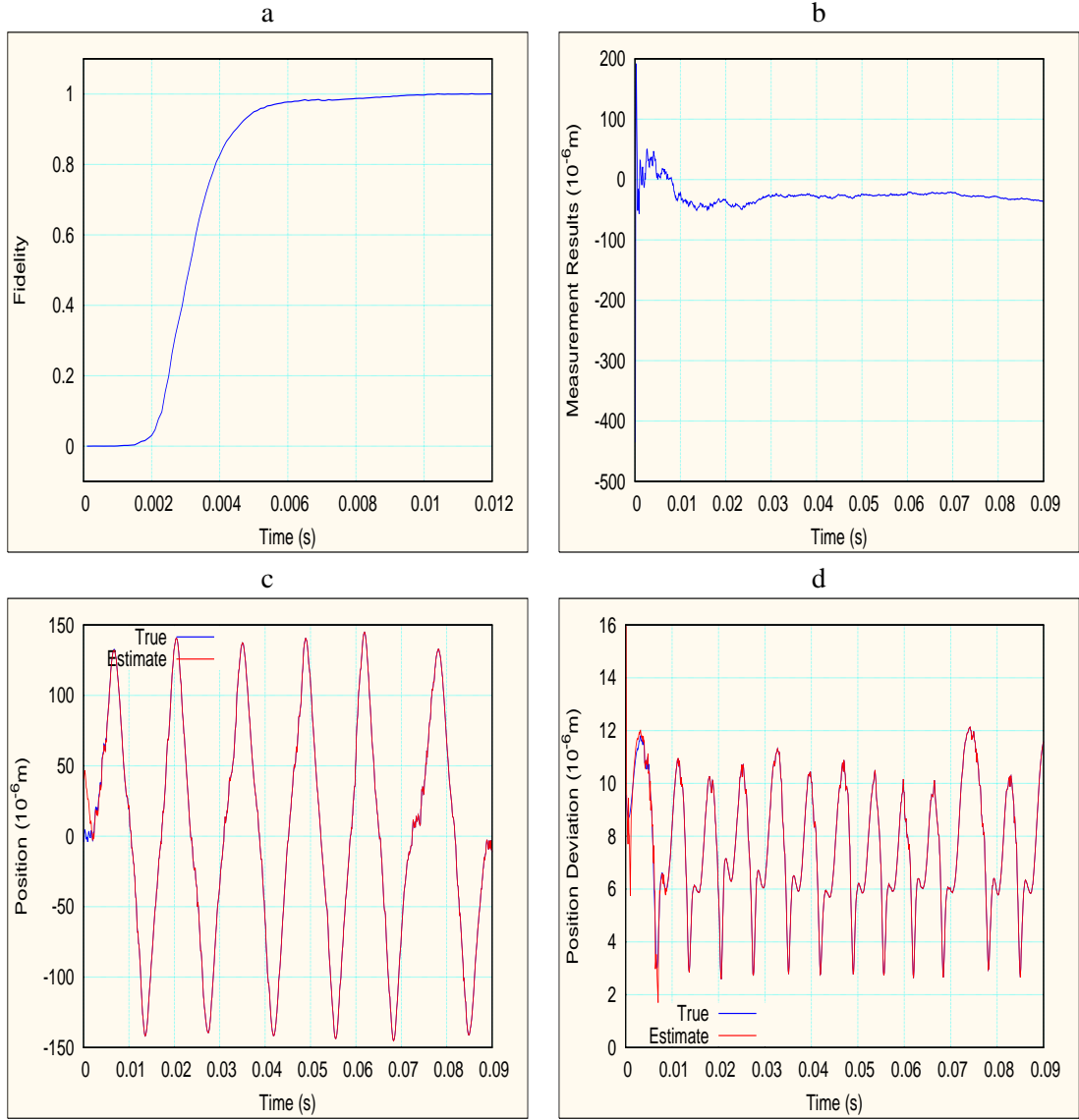


Figure 5.7: Results of the simulation of the evolution of the one dimensional wave function of a hydrogen atom in a double well potential whose position is continuously monitored. a) The evolution of fidelity with time. b) The variation of averaged measurement results with time. c) The variation of the mean position of the atom with time. d) The variation of the deviation of position with time.

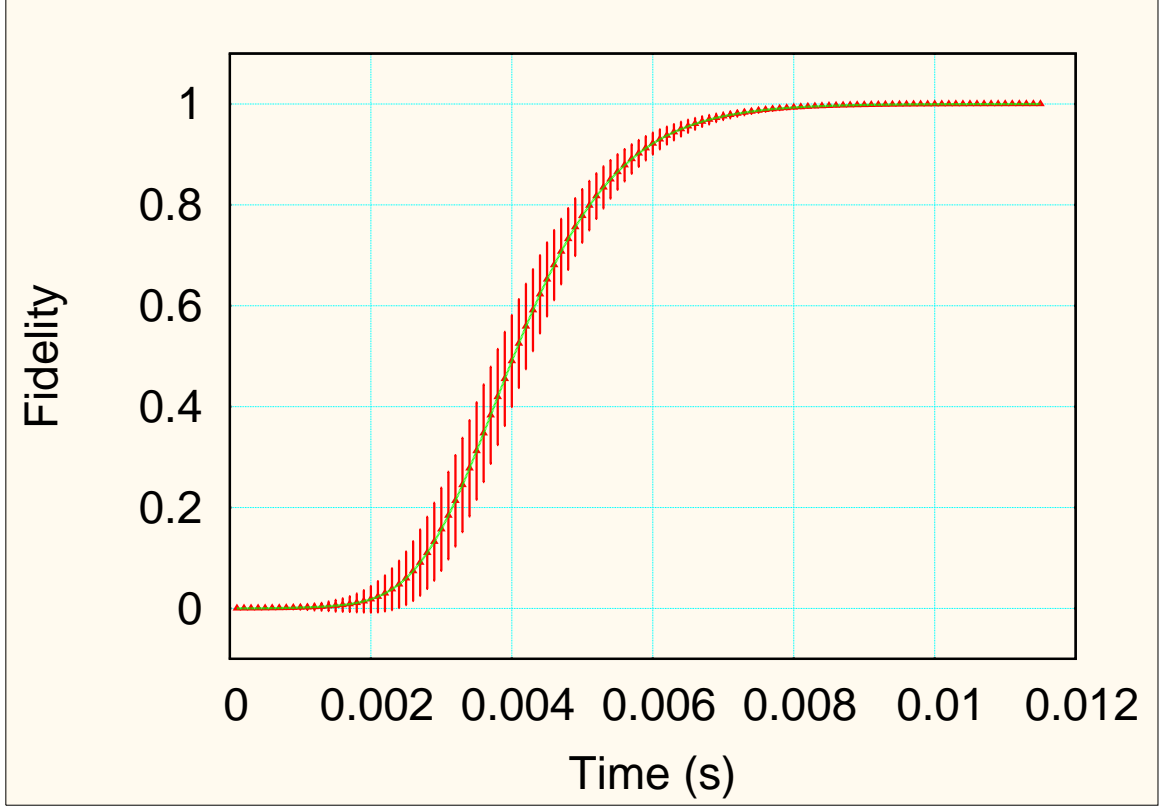


Figure 5.8: The variation of average fidelity (with error bars) with time for a free hydrogen atom.

expression:

$$\log_{10} t_c = \mu \log_{10} \gamma + \kappa, \quad (5.68)$$

where μ and κ are constants. Raising both sides of equation (5.68) to base 10, we obtain the following:

$$\begin{aligned} t_c &= 10^{\mu \log_{10} \gamma + \kappa} \\ &= 10^\kappa \gamma^\mu \\ &= \alpha \left(\frac{\gamma}{\beta} \right)^\mu, \end{aligned} \quad (5.69)$$

where $\alpha/\beta^\mu = 10^\kappa$, β is a constant with the units of γ and α is a constant with units of time. To test relation (5.69), we fitted the convergence data for the free hydrogen atom to the equation using the Marquardt-Levenberg algorithm provided in Gnuplot and generated the blue line in fig 5.11, thus confirming the power law. For this case the constants κ and μ were calculated to be -0.455965

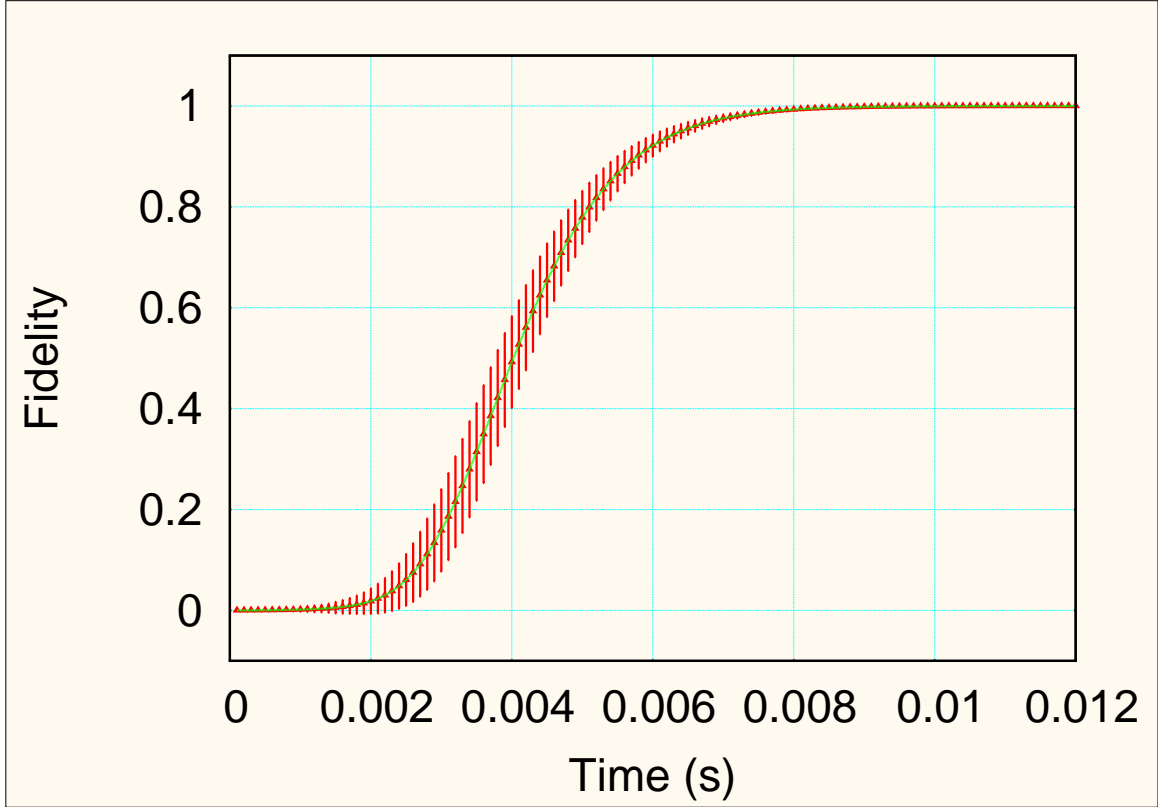


Figure 5.9: The variation of average fidelity (with error bars) with time for a hydrogen atom in the harmonic potential.

and 3.84223 respectively. In future, in order to obtain more accurate values of κ and μ , mean data from several runs of the simulation will be used as was done by Konrad and Uys. It would also be interesting, in the future, to see how α , β and μ will vary if we vary the several free parameters in stochastic differential equations and also to verify if the speculated power law holds in cases where the atom is bounded in different potentials.

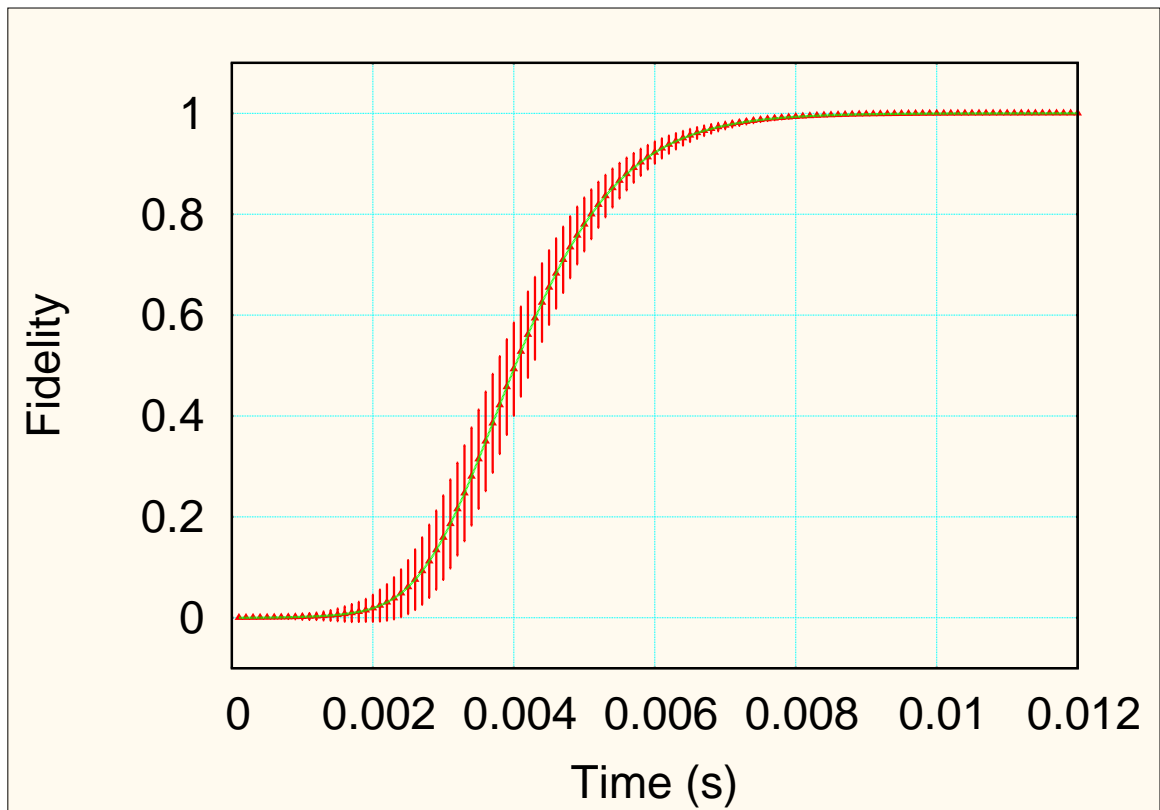


Figure 5.10: The variation of average fidelity (with error bars) with time for a hydrogen atom in the double well potential.

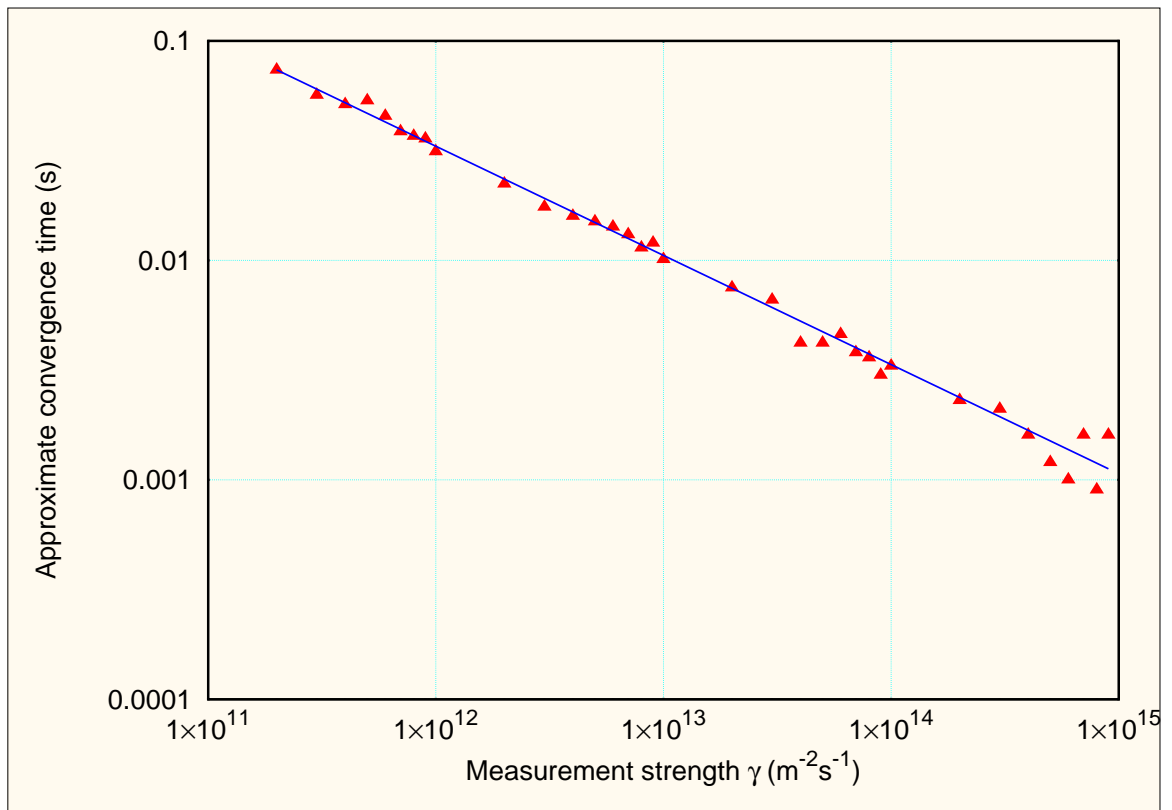


Figure 5.11: The variation of convergence time t_c with the measurement strengths γ for a free particle.

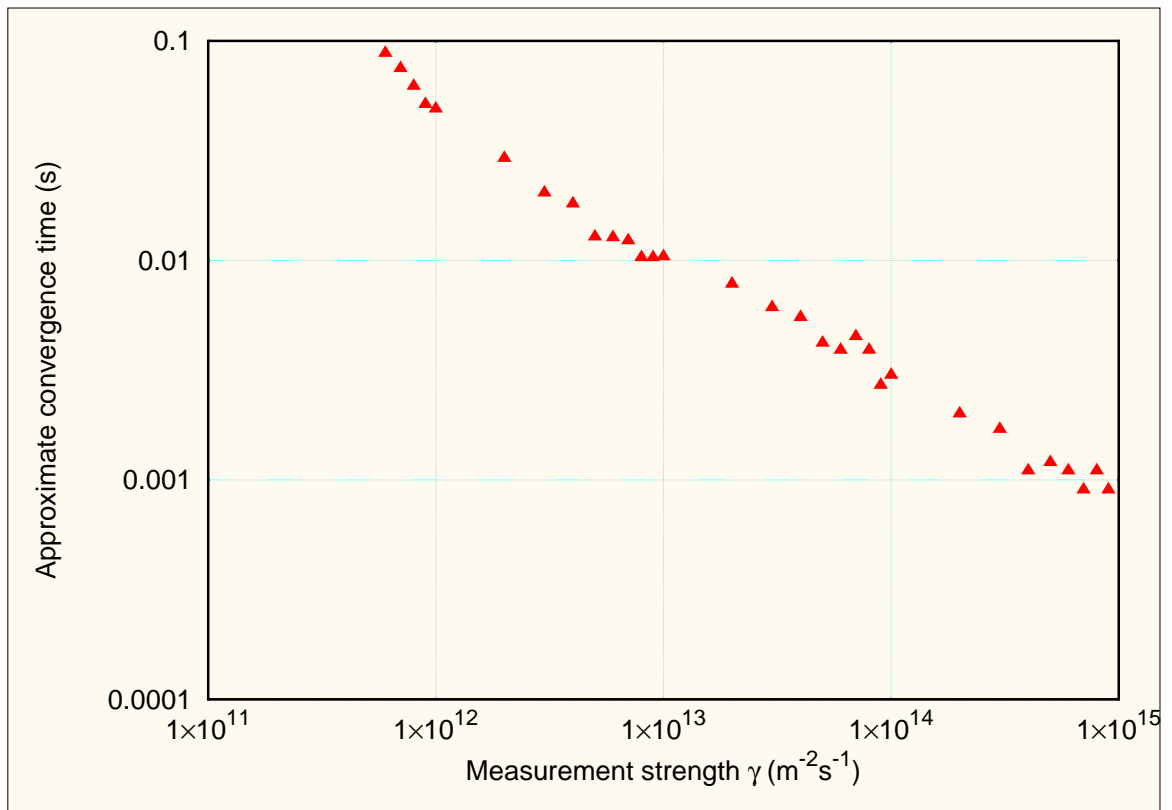


Figure 5.12: The variation of convergence time t_c with the measurement strengths γ for a particle in the harmonic potential.

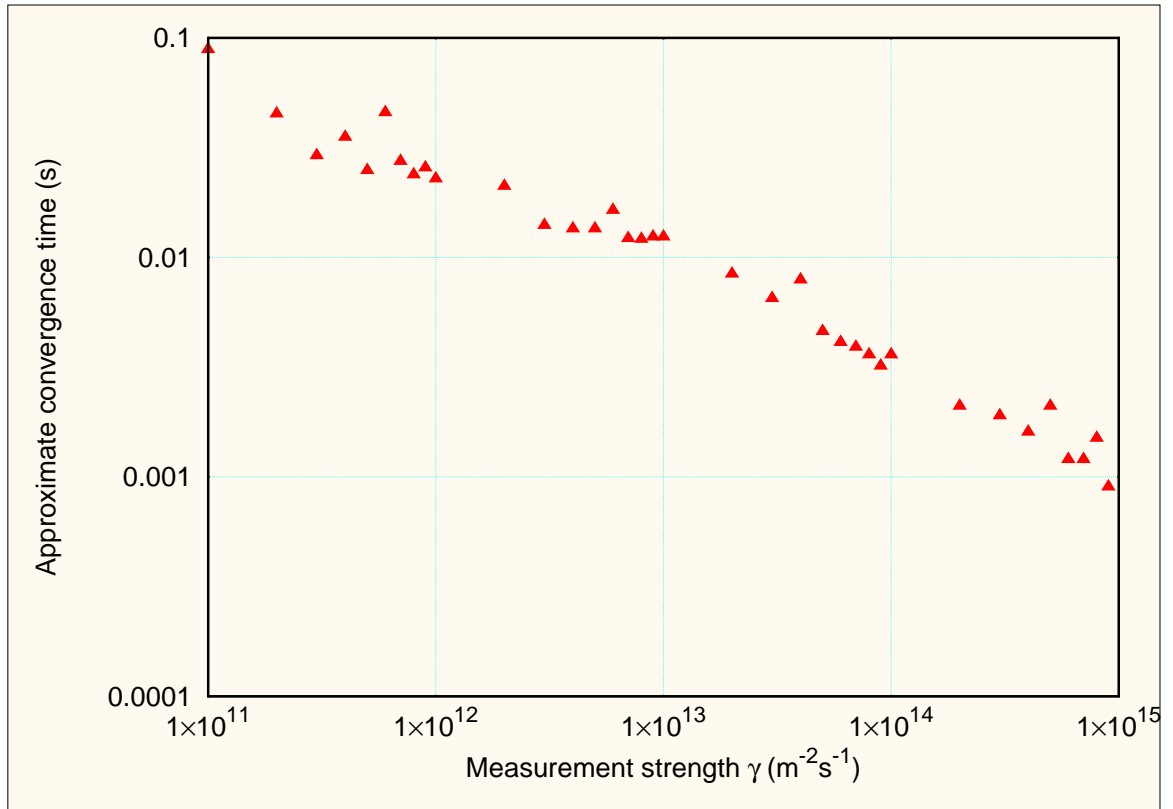


Figure 5.13: The variation of convergence time t_c with the measurement strengths γ for a particle in the double well potential.

Chapter 6

Conclusion and Outlook

6.1 Conclusion

Continuous monitoring of the position of a single quantum system is possible. In this thesis we showed that a scheme, which involves initially estimating the state (wave function) and then updating it using integrated results from a quick succession of unsharp position measurements can be used for this purpose. From the numerical simulations it is conclusive that given enough time the estimated wave function converges to the true wave function, and the dynamics of the estimated wave function effectively describes the dynamics of the system. In fact, one of the major highlights of the work presented in this thesis was the discovery, through numerics, of the power law variation of convergence time with measurement strengths for the free particle, with the results for the particle trapped in the harmonic and double well potentials suggesting a similar variation. This is a great leap forward in that such a law provides an experimenter with a tool that enables him to reasonably estimate the amount of time required for the estimated state to converge to the true one; that is, it makes ‘enough time’ quantifiable.

The monitoring scheme is mathematically described by three coupled Ito stochastic differential equations: one that describes the evolution of the true state of the system (equation (3.53)), one that describes the evolution of the integrated measurement results (equation (3.39)) and one that describes the evolution of the estimated state (equation (4.17)). We went a step further from just borrowing these equations from the sources in which they were first published (the first two can be found in [14] and the last one in [15]) to providing an alternative, and quite simplified, way to derive these equations from basic quantum mechanics, through the application of generalized position observables (represented by positive operator-valued measures), and not standard position measurements, which are described by the collapse of the wave function. In fact generalized measurement theory provides a more accurate description of the quantum measurement process, and is mathematically plausible because it is derived from the theory of measures.

6.2 Outlook

Moving forward, the most immediate task would be to probe the convergence law further. Whilst in this thesis we have exercised the liberty to vary just the measurement strengths in order to determine the convergence law, it is important to know how the parameters given in the law vary with the other experimental parameters. In doing so we come up with an explicit law which enables the experimenter to accurately approximate the convergence time, given his or her experimental set up.

The second task would be to expand the numerical simulations to 2- and eventually 3-dimensional spaces. To achieve this it would require solving the problem of numerics from a computational point of view, with a goal of improving performance. This would involve the use of transformations and advanced computing algorithms in conjunction with high performance computing platforms, such as message passing interface (MPI) or graphics programming units (GPU's).

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Appendix A

One dimensional source code

constants.h

```
#ifndef CONSTANTS_H
#define CONSTANTS_H
/*=====*/
/* Include some header files here */
/*=====*/
#include <math.h>
/*=====*/
/* Define some constants here */
/*=====*/
#define A (1 / sqrt(sqrt(2 * PI * sx * s * sx * s)))
#define Ae (1 / sqrt(sqrt(2 * PI * sxe * s * sxe * s)))
#define sx 5
#define sxe 5
#define kx 0
#define kxe 0
#define xglo -200
#define xgup 200
#define xglo (xglo - xres)
#define xgup (xgup + xres)
#define xlower (xglo - 2 * xres)
#define xupper (xgup + 2 * xres)
#define x0 0
#define x0e 50
#define xsize ((xupper - xlower) / xres + 1)
#define PI 3.14159265
#define s 1e-6
#define dx (xres * s)
#define end 100001
#define gx (1 / (sigma_x * sigma_x * tau)) / (sigma_x * sqrt(tau))
#define sigma_x 1e-5
#define sigma_y 1e-5
#define tau 1e-4
#define ELECTRONMASS 9.1093897e-31
#define dt 5e-8
#define HBAR 1.05457266e-34
#define m (PROTONMASS + ELECTRONMASS)
```

```

#define PI 3.14159265
#define progress 500
#define PROTONMASS 1.6726231e-27
#define qx (dx / s)
#define qx2 (sqrt(dt) / (sqrt(gx))) //(sqrt(dt) / (gx * dt))
#define record 50
#define xres 1
#define ux1 (I * HBAR * dt / (2 * m * dx * dx))
#define ul (I * HBAR / (2 * m))
#define u2 (I * m * dt / HBAR)
#define mx1 (dt * dx * dx * gx / 8) //(dt * dx * dx / (8 * gx * gx))
#define mx2 (dx * sqrt(dt) * sqrt(gx) / 2) //(dx * sqrt(dt) / (2 * gx))
#define mx3 (sqrt(dt) * dx * sqrt(gx)) //(sqrt(dt) * dx / gx)
#define width 52
#define height 3
#define rows 25
#define cols 80
#define px ((cols - width) / 2)
#define py ((rows - height) / 2)
#define px1 px
#define py1 (py - 10)
#define px2 (px + 23)
#define py2 (py + 3)
/*=====*/
#endif

```

main.c

```

/*
COMMENT: This file contains the main function of the program...
*/
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <complex.h>
#include "constants.h"
int main(int argc, char *argv[])
{
    /*=====*/
    /* Declaration of variables */
    /*=====*/
    _Complex double *psi;
    _Complex double *psie;
    double *pot;
    long t1, t2;
    /*=====*/
    /* Declaration of functions */
    /*=====*/
    void plot_phase_wavefunction();
    void plot_data();
    void make_movie();
    void record_initial(_Complex double *phi, _Complex double *phie);
    void initialize(_Complex double *phi, _Complex double *phie, double *pot);
    void prog_done();
    void second_order_weak(_Complex double *phi, _Complex double *phie, double *pot);
    /*=====*/
}

```

```

/* Dynamic allocation of memory for wave function and potential array */
/*=====*/
psi = malloc(xsize * sizeof(_Complex double));
psie = malloc(xsize * sizeof(_Complex double));
pot = malloc(xsize * sizeof(double));
if(psi == NULL || psie == NULL || pot == NULL)
{
    fprintf(stderr, "out of memory\n");
    exit(EXIT_FAILURE);
}
/*=====*/
/* Call functions to the Simulation */
/*=====*/
//system("make clean");
t1 = time(NULL);
//initialize(psi, psie, pot);
//record_initial(psi, psie);
//second_order_weak(psi, psie, pot);
//plot_phase_wavefunction();
//plot_data();
make_movie();
/*=====*/
/* Free memory */
/*=====*/
free(psi);
free(psie);
free(pot);
/*=====*/
/* Done!!! */
/*=====*/
t2 = time(NULL);
printf("\n total time: %ld\n", t2 - t1);
prog_done();
return 0;
/*=====*/
}

```

initialize.c

```

/*
COMMENT: This file contains the function that initializes the wave functions and the potential...
*/
#include "constants.h"
#include <stdlib.h>
#include <stdio.h>
#include <complex.h>
void initialize(_Complex double *phi, _Complex double *phie, double *pot)
{
    /*=====*/
    /* Declare and initialize variables */
    /*=====*/
    int x, y;
    double prob = 0.0, probe = 0.0;
    /*=====*/
    /* Initialize wave functions and potential*/
    /*=====*/
}

```

```

for(x = xlower; x <= xupper; x += xres)
{
    phi[(x - xlower) / xres]
    = A * cexp(-I * kx * x * s - (x - x0) * s * (x - x0) * s / (4 * sx * s * sx * s));
    phie[(x - xlower) / xres]
    = Ae * cexp(-I * kxe * x * s - (x - x0e) * s * (x - x0e) * s / (4 * sxe * s * sxe * s));
    pot[(x - xlower) / xres] = 0.5 * m * le6 * x * s * x * s;
    prob += dx * cabs(phi[(x - xlower) / xres]) * cabs(phi[(x - xlower) / xres]);
    probe += dx * cabs(phie[(x - xlower) / xres]) * cabs(phie[(x - xlower) / xres]);
}
/*****

```

second_order_weak.c

```

/*
    COMMENT: This file contains the function that simulates the dynamics
             of the wave functions using the second order weak scheme...
*/
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <complex.h>
#include <time.h>
#include <omp.h>
#include "constants.h"
#include <curses.h>
void second_order_weak(_Complex double *phi, _Complex double *phie, double *pot)
{
    /*****
    /* Declaration of variables */
    /*****
    _Complex double *dummyphi;
    _Complex double *dummyphie;
    _Complex double *phi_t;
    _Complex double *phi_m;
    _Complex double *phi_p;
    _Complex double *phie_m;
    _Complex double *phie_p;
    _Complex double *phie_t;
    _Complex double part1, part2t, part2pm;
    char datafile[500];
    char phasefile[500];
    double norm_t, norm_p, norm_m;
    double norme_t, norme_p, norme_m;
    double xb, xbe;
    double norm, norme;
    double fidelity, finalfid;
    double varx, varxe;
    double deviation, deviation_e;
    double ranx, rany;
    double Qx, mqx;
    FILE *p9;
    int ixp1, ixp2, ixp3, ix, x;
    int ixc, ixl, ixr;
    int tstep;

```

```

long seedx = 0 - (long)time(NULL);
/*****
/* Declataion of functions which are called in this function */
/*****
void clean_up();
void current_progress(int step);
void initial_progress();
double gasdev(long *idum);
void create_files();
void pfreord(_Complex double *phi, _Complex double *phie, int tmstp);
void frecord1(int timestep, double xbar, double xbare, double fidelity, double varx,
double varxe, double devx, double devxe, double mx);
void calc_norm_all(_Complex double *phi_t, _Complex double *phi_p, _Complex double *phi_m,
_Complex double *phie_t, _Complex double *phie_p, _Complex double *phie_m,
double *normt, double *normp, double *normm, double *normet,
double *normep, double *normem);
void calc_quant_all(_Complex double *phi, _Complex double *phie, double *ab, double *ab2,
double *abe, double *abe2, double *fid, double *nm, double *nme);
/*****
/* Allocate memory using malloc() */
/*****
dummyphi = malloc((xsize - 4) * sizeof(_Complex double));
dummyphie = malloc((xsize - 4) * sizeof(_Complex double));
phi_m = malloc((xsize - 2) * sizeof(_Complex double));
phi_p = malloc((xsize - 2) * sizeof(_Complex double));
phi_t = malloc((xsize - 2) * sizeof(_Complex double));
phie_m = malloc((xsize - 2) * sizeof(_Complex double));
phie_p = malloc((xsize - 2) * sizeof(_Complex double));
phie_t = malloc((xsize - 2) * sizeof(_Complex double));
if(dummyphi == NULL || dummyphie == NULL || phi_m == NULL || phi_p == NULL || phi_t == NULL ||
phie_m == NULL || phie_p == NULL || phie_t == NULL)
{
    fprintf(stderr, "out of memory\n");
    exit(EXIT_FAILURE);
}
/*****
/* Display initial progress */
/*****
initial_progress();
/*****
/* Second Order Weak Scheme*/
/*****
create_files();
tstep = 1;
Qx = 0;
while(tstep < end)
{
    ranx = gasdev(&seedx);
    calc_quant_all(phi, phie, &xb, &varx, &xbe, &varxe, &fidelity, &norm, &norme);
    Qx += (qx * xb + qx2 * ranx);
    /*
    * COMMENT: Display the progress of the program at pre-defined intervals
    */
    if((tstep%progress) == 0)
    {
        current_progress(tstep);
    }
}

```

```

}

/*
 *      COMMENT: Record quantities to data files...
 */
if((tstep%record) == 0)
{
    mqx = Qx / tstep;
    frecord1(tstep, xb, xbe, fidelity, varx, varxe, sqrt(varx), sqrt(varxe), mqx);
    pfrecord(phi, phie, tstep);
}

/*
 *      COMMENT: Calculate the tilde values...
 *      ixc and iyc are the indices of the central values
 */
for(ixc = 1; ixc <= xgupt - xglot + 1; ixc += xres)
{
    /*
     *      COMMENT: Indices to dereference the phi and phie arrays...
     */
    ixl = ixc - 1; // starts at memory address 0
    ixr = ixc + 1; // starts at memory address 2

    part1
    = phi[ixc] / norm
    + ux1 * (phi[ixl] + phi[ixr] - 2 * phi[ixc]) / norm
    - u2 * pot[ixc] * phi[ixc] / norm
    - mx1 * (x - xb) * (x - xb) * phi[ixc] / norm;
    part2t
    = mx2 * (x - xb) * phi[ixc] / norm * ranx;
    part2pm
    = mx2 * (x - xb) * phi[ixc] / norm;
    phi_t[ixl] = part1 + part2t;
    phi_p[ixl] = part1 + part2pm;
    phi_m[ixl] = part1 - part2pm;

    part1
    = phie[ixc] / norme
    + ux1 * (phie[ixl] + phie[ixr] - 2 * phie[ixc]) / norme
    - u2 * pot[ixc] * phie[ixc] / norme
    - mx1 * (x - xbe) * (x - xbe) * phie[ixc] / norme;
    part2t
    = mx2 * (x - xbe) * phie[ixc] / norme * ranx;
    part2pm
    = mx2 * (x - xbe) * phie[ixc] / norme;
    phie_t[ixl] = part1 + part2t;
    phie_p[ixl] = part1 + part2pm;
    phie_m[ixl] = part1 - part2pm;
}

/*
 *      COMMENT: Calculate the norms of the tilde wave functions...
 */
calc_norm_all(phi_t, phi_p, phi_m, phie_t, phie_p, phie_m, &norm_t,
&norm_p, &norm_m, &norme_t, &norme_p, &norme_m);

```



```

/*
 *      COMMENT: Calculate the new wave functions...
 */
for(x = xglo; x <= xgup; x += xres)
{
    ix = (x - xglo) / xres;
    ixp1 = (x - xglo) / xres + 1;
    ixp2 = (x - xglo) / xres + 2;
    ixp3 = (x - xglo) / xres + 3;

    dummyphi[ix]
    = phi[ixp2] / norm
    + 0.5 * (ux1 * ((phi[ixp1] + phi[ixp3] - 2 * phi[ixp2]) / norm
    + (phi_t[ix] + phi_t[ixp2] - 2 * phi_t[ixp1]) / norm_t)
    - u2 * pot[ixp2] * (phi[ixp2] / norm + phi_t[ixp1] / norm_t)
    - mx1 * (x - xb) * (x - xb) * (phi[ixp2] / norm + phi_t[ixp1] / norm_t))
    + 0.25 * (mx2 * (x - xb) * (phi_p[ixp1] / norm_p + phi_m[ixp1] / norm_m
    + 2 * phi[ixp2] / norm) * ranx)
    + 0.25 * (mx2 * (x - xb) * (phi_p[ixp1] / norm_p
    - phi_m[ixp1] / norm_m) * ((ranx * ranx) - 1)));

    dummyphie[ix]
    = phie[ixp2] / norme
    + 0.5 * (ux1 * ((phie[ixp1] + phie[ixp3] - 2 * phie[ixp2]) / norme
    + (phie_t[ix] + phie_t[ixp2] - 2 * phie_t[ixp1]) / norme_t)
    - u2 * pot[ixp2] * (phie[ixp2] / norme + phie_t[ixp1] / norme_t)
    - mx1 * (x - xb) * (x - xb) * (phie[ixp2] / norme + phie_t[ixp1] / norme_t))
    + 0.25 * (mx2 * (x - xb) * (phie_p[ixp1] / norme_p + phie_m[ixp1] / norme_m
    + 2 * phie[ixp2] / norme) * (ranx + mx3 * (xb - xbe)))
    + 0.25 * (mx2 * (x - xb) * (phie_p[ixp1] / norme_p
    - phie_m[ixp1] / norme_m) * ((ranx + mx3 * (xb - xbe)
    * (ranx + mx3 * (xb - xbe)) - 1)));
}
/*
 *      COMMENT: Update our wave functions...
 */
for(x = xglo; x <= xgup; x += xres)
{
    ix = (x - xglo) / xres;
    ixp2 = (x - xglo) / xres + 2;

    phi[ixp2] = dummyphi[ix];
    phie[ixp2] = dummyphie[ix];
}
tstep++;
}
/*=====*/
/* Clean up */
/*=====*/
clean_up();
free(phi_m);
free(phie_m);
free(phi_p);
free(phie_p);
free(phi_t);

```

```

    free(phie_t);
    free(dummyphi);
    free(dummyphie);
    /*=====*/
}

```

ran1.c

```

/*
COMMENT: This file was obtained from NUMERICAL RECIPES...
         It is works in conjunction with "gasdev.c"...
*/

```

```

#define IA 16807
#define IM 2147483647
#define AM (1.0/IM)
#define IQ 127773
#define IR 2836
#define NTAB 32
#define NDIV (1+(IM-1)/NTAB)
#define EPS 1.2e-7
#define RNMX (1.0-EPS)

float ran1(long *idum)
{
    int j;
    long k;
    static long iy=0;
    static long iv[NTAB];
    float temp;

    if (*idum <= 0 || !iy) {
        if (-(*idum) < 1) *idum=1;
        else *idum = -(*idum);
        for (j=NTAB+7;j>=0;j--) {
            k=(*idum)/IQ;
            *idum=IA*(*idum-k*IQ)-IR*k;
            if (*idum < 0) *idum += IM;
            if (j < NTAB) iv[j] = *idum;
        }
        iy=iv[0];
    }
    k=(*idum)/IQ;
    *idum=IA*(*idum-k*IQ)-IR*k;
    if (*idum < 0) *idum += IM;
    j=iy/NDIV;
    iy=iv[j];
    iv[j] = *idum;
    if ((temp=AM*iy) > RNMX) return RNMX;
    else return temp;
}
#undef IA
#undef IM
#undef AM
#undef IQ
#undef IR

```

```
#undef NTAB
#undef NDIV
#undef EPS
#undef RNMX
```

gasdev.c

```
/*
COMMENT: This file was obtained from NUMERICAL RECIPES...
        It works in conjunction with the file "ran1.c"
        to generate Gaussian distributed random numbers...
*/
#include <math.h>

float gasdev(long *idum)
{
    float ran1(long *idum);
    static int iset=0;
    static float gset;
    float fac,rsq,v1,v2;

    if (*idum < 0) iset=0;
    if (iset == 0) {
        do {
            v1=2.0*ran1(idum)-1.0;
            v2=2.0*ran1(idum)-1.0;
            rsq=v1*v1+v2*v2;
        } while (rsq >= 1.0 || rsq == 0.0);
        fac=sqrt(-2.0*log(rsq)/rsq);
        gset=v1*fac;
        iset=1;
        return v2*fac;
    } else {
        iset=0;
        return gset;
    }
}
```

calc_norm_t.c

```
/*
COMMENT: This files contains the function that calculates
        the norms of our tilde wave functions...
        It makes use of lots of pointers to
        pass variables by reference...
*/
#include "constants.h"
#include <math.h>
#include <stdlib.h>
#include <complex.h>
void calc_norm_all(_Complex double *phi_t, _Complex double *phi_p, _Complex double *phi_m,
    _Complex double *phie_t, _Complex double *phie_p, _Complex double *phie_m,
    double *normt, double *normp, double *normm,
    double *normet, double *normep, double *normem)
{
```

```

/*=====*/
/* Declare variables */
/*=====*/
int x;
/*=====*/
/* Initialize variables */
/*=====*/
*normt = 0.0;
*normp = 0.0;
*normm = 0.0;
*normet = 0.0;
*normep = 0.0;
*normem = 0.0;
/*=====*/
/* Calculate quantities */
/*=====*/
for(x = xglot; x <= xgupt; x += xres)
{
    *normt += dx * cabs(phi_t[(x - xglot) / xres]) * cabs(phi_t[(x - xglot) / xres]);
    *normp += dx * cabs(phi_p[(x - xglot) / xres]) * cabs(phi_p[(x - xglot) / xres]);
    *normm += dx * cabs(phi_m[(x - xglot) / xres]) * cabs(phi_m[(x - xglot) / xres]);
    *normet += dx * cabs(phie_t[(x - xglot) / xres]) * cabs(phie_t[(x - xglot) / xres]);
    *normep += dx * cabs(phie_p[(x - xglot) / xres]) * cabs(phie_p[(x - xglot) / xres]);
    *normem += dx * cabs(phie_m[(x - xglot) / xres]) * cabs(phie_m[(x - xglot) / xres]);
}
*normt = sqrt(*normt);
*normp = sqrt(*normp);
*normm = sqrt(*normm);
*normet = sqrt(*normet);
*normep = sqrt(*normep);
*normem = sqrt(*normem);
/*=====*/
}

```

calc_quantities.c

```

/*
COMMENT: This file contains the function that computes the following quantities
        (Given the true and estimated wave functions):
        fidelity, norm, mean position and position variance...
        NOTE: It makes use of lots of pointers to pass variables by reference...
*/
#include "constants.h"
#include <stdlib.h>
#include <complex.h>
#include <omp.h>
void calc_quant_all(_Complex double *phi, _Complex double *phie, double *ab, double *ab2,
    double *abe, double *abe2, double *fid, double *nm, double *nme)
{
    /*=====*/
    /* Declare and initialize variables */
    /*=====*/
    _Complex double fidelity = 0.0;

```

```

double prob;
double probe;
int x, y;
*nm = 0.0;
*nme = 0.0;
*ab = 0.0;
*abe = 0.0;
*ab2 = 0.0;
*abe2 = 0.0;
/*=====*/
/* Calculate quantities */
/*=====*/
for(x = xglo; x <= xgup; x += xres)
{
    prob = cabs(phi[(x - xlower) / xres]) * cabs(phi[(x - xlower) / xres]);
    probe = cabs(phie[(x - xlower) / xres]) * cabs(phie[(x - xlower) / xres]);
    *nm += dx * prob;
    *nme += dx * probe;
    *ab += x * dx * prob;
    *abe += x * dx * probe;
    *ab2 += x * x * dx * prob;
    *abe2 += x * x * dx * probe;
    fidelity += conj(phie[(x - xlower) / xres]) * phi[(x - xlower) / xres] * dx;
}
*nm = sqrt(*nm);
*nme = sqrt(*nme);
*ab2 -= (*ab)*(*ab);
*abe2 -= (*abe)*(*abe);
*fid = cabs(fidelity) * cabs(fidelity);
/*=====*/
}

```

graphics.c

```

/*
COMMENT: This file contains functions that display the progress
on the console...
*/

#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <complex.h>
#include <omp.h>
#include "constants.h"
#include <curses.h>
/*=====*/
/* Variable declaration for progress display */
/*=====*/
WINDOW * mainwin, * childwin, * childwin1, * childwin2;
int ch;
char prog[50], prog1[20];
int pind;
int tempp, percent = 0;
int flag = 0;

```

```

/*=====*/
void initial_progress()
{
    /*=====*/
    /* Display initial progress */
    /*=====*/
    strcpy(prog, ""); //Necessary... To assign an empty string to the variable prog...
    if ((mainwin = initscr()) == NULL)
    {
        fprintf(stderr, "Error initialising ncurses.\n");
        exit(EXIT_FAILURE);
    }
    start_color();
    if(has_colors())
    {
        init_pair(8, COLOR_WHITE, COLOR_RED);
    }
    childwin2 = subwin(mainwin, 3, 6, py2, px2);
    box(childwin2, 0, 0);
    childwin1 = subwin(mainwin, 10, width, py1, px1);
    box(childwin1, 0, 0);
    mvwaddstr(childwin1, 2, 10, "Stochastic Simulation Ver. final");
    mvwaddstr(childwin1, 3, 14, "Written by Kevin Garapo");
    mvwaddstr(childwin1, 4, 12, "As part of Masters Research");
    mvwaddstr(childwin1, 5, 11, "At University of KwaZulu-Natal");
    mvwaddstr(childwin1, 6, 16, "(c) February 2011");
    mvwaddstr(childwin1, 7, 11, "email: kevingarapo@gmail.com");
    color_set(8, NULL);
    childwin = subwin(mainwin, height, width, py, px);
    box(childwin, 0, 0);
    mvaddstr(py2 + 1, px2 + 4, "%");
    for(pind = 1; pind <= 1; pind++)
    {
        strcat(prog, "");
        sprintf(progl, "%3d", 0 * pind * 2);
        mvaddstr(py2 + 1, px2 + 1, progl);
        refresh();
        mvaddstr(py + 1, px + 1, prog);
        refresh();
        mvaddstr(1, 1, "");
        refresh();
    }
    /*=====*/
}

void current_progress(int step)
{
    /*=====*/
    /* Display the progress of the program at pre-defined intervals */
    /*=====*/
    if((step%progress) == 0)
    {
        tempp = (int)(100 * step / (end - 1));
        if((tempp % 2) != 0 )
        {
            tempp -= 1;

```

```

        flag = 1;
    }
    if(tempp > percent)
    {
        for(pind = percent; pind < tempp; pind += 2)
        {
            strcat(prog, " ");
        }
        mvaddstr(py + 1, px + 1, prog);
        refresh();
    }
    sprintf(progl,"%3d", tempp + flag);
    mvaddstr(py2 + 1, px2 + 1, progl);
    refresh();
    mvaddstr(1, 1, "");
    refresh();
    flag = 0;
    percent = tempp;
}
/*=====*/
}

void clean_up()
{
    /*=====*/
    /* Clean up display */
    /*=====*/
    delwin(childwin);
    delwin(childwin1);
    delwin(childwin2);
    delwin(mainwin);
    endwin();
    refresh();
    /*=====*/
}

```

create_files.c

```

/*
COMMENT: This file contains the function that
         creates the data files to store plot data....
*/
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <complex.h>
#include <time.h>
#include "constants.h"

void create_files()
{
    /*=====*/
    /* Declare variables */
    /*=====*/
    FILE *p1, *p2, *p3, *p4, *p5, *p6, *p7, *p8;
}

```

```

/*=====*/
/* Create data files and close them */
/*=====*/
p1=fopen("quantitative/mean.dat","wb");
p2=fopen("quantitative/mean1.dat","wb");
p3=fopen("quantitative/fidelity.dat","wb");
p4=fopen("quantitative/variance.dat","wb");
p5=fopen("quantitative/variance1.dat","wb");
p6=fopen("quantitative/stddev.dat","wb");
p7=fopen("quantitative/stddev1.dat","wb");
p8=fopen("quantitative/results.dat","wb");
fclose(p1);
fclose(p2);
fclose(p3);
fclose(p4);
fclose(p5);
fclose(p6);
fclose(p7);
fclose(p8);
/*=====*/
}

```

record.c

```

/*
COMMENT: This file contains the function that records
         wave functions and phases to data files...
*/
#include "constants.h"
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <complex.h>
void pfreord(_Complex double *phi, _Complex double *phie, int tmstp)
{
    /*=====*/
    /* Declare and initialize variables */
    /*=====*/
    char dtfile[500];
    char dtfile1[500];
    FILE *fp, *fp1;
    int x, flag = 0, flag1 = 0;
    /*=====*/
    /* Open data files, record data and close */
    /*=====*/
    sprintf(dtfile, "wavefunction/data%.6d.dat", tmstp);
    sprintf(dtfile1, "phase/data%.6d.dat", tmstp);
    fp = fopen(dtfile,"wb");
    fp1 = fopen(dtfile1,"wb");
    for(x = xglo; x <= xgup; x += xres)
    {
        fprintf(fp,"%d\t%f\t%f\n", x, cabs(phi[(x - xlower) / xres]) * cabs(phi[(x - xlower) / xres]),
            cabs(phie[(x - xlower) / xres]) * cabs(phie[(x - xlower) / xres]));
        if(cabs(phi[(x - xlower) / xres]) < 1e-3 && cabs(phie[(x - xlower) / xres]) < 1e-3)
            fprintf(fp1,"%d\t%f\t%f\n", x, 0.0, 0.0);
        else if(cabs(phi[(x - xlower) / xres]) < 1e-3 && cabs(phie[(x - xlower) / xres]) > 1e-3)

```



```

        fprintf(fp1,"%d\t%f\t%f\n", x, 0.0,
        fmod(carg(phie[(x - xlower) / xres]) / cabs(phie[(x - xlower) / xres]), 2 * PI));
    else if(cabs(phi[(x - xlower) / xres]) > 1e-3 && cabs(phie[(x - xlower) / xres]) < 1e-3)
        fprintf(fp1,"%d\t%f\t%f\n", x,
        fmod(carg(phi[(x - xlower) / xres]) / cabs(phi[(x - xlower) / xres]), 2 * PI), 0.0);
    else
        fprintf(fp1,"%d\t%f\t%f\n", x,
        fmod(carg(phi[(x - xlower) / xres]) / cabs(phi[(x - xlower) / xres]), 2 * PI),
        fmod(carg(phie[(x - xlower) / xres]) / cabs(phie[(x - xlower) / xres]), 2 * PI));
    }
    fclose(fp);
    fclose(fp1);
    /*****
}

```

plots_and_movies.c

```

/*
COMMENT: This file contains the functions that plots data
        using GNUPLOT and generates movies using ffmpeg...
*/
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <complex.h>
#include <omp.h>
#include "constants.h"
void plot_phase_wavefunction()
{
    /*****
    /* Declare variables */
    /*****
    char dtfile[500];
    char dtfile1[500];
    char outfile[500];
    char outfile1[500];
    FILE *gnuplotPipe;
    int x;
    /*****
    /* Open pipe, plot data using Gnuplot and close */
    /*****
    printf("Plotting data...\n");
    for(x = 0; x < end; x += record)
    {
        gnuplotPipe = popen("gnuplot -persist","w");
        if (gnuplotPipe)
        {
            fprintf(gnuplotPipe, "set style data lines\n");
            fprintf(gnuplotPipe, "set border 31 lw 2\n");
            fprintf(gnuplotPipe, "set style line 1 lt 1 lw 3\n");
            fprintf(gnuplotPipe, "set style line 2 lt 2 lw 3\n");
            fprintf(gnuplotPipe, "set style line 3 lt 3 lw 3\n");
            fprintf(gnuplotPipe, "set key box linestyle 1\n");
            fprintf(gnuplotPipe,
                "set terminal jpeg enhanced font \"FreeSansOblique.ttf,40\" size 1500,1500\n");
            fprintf(gnuplotPipe, "set xrange [%d:%d]\n", xlower, xupper);

```

```

        sprintf(dtfile, "wavefunction/data%.6d.dat", x);
        sprintf(dtfile1, "phase/data%.6d.dat", x);
        sprintf(outfile, "wavefunction/%.6d.jpeg", x / record);
        sprintf(outfile1, "phase/%.6d.jpeg", x / record);
        fprintf(gnuplotPipe, "set label '%0.6fs' at 10,150000 center textcolor lt 1\n",
(float)x * dt);
        fprintf(gnuplotPipe, "set xlabel 'Distance (10^{%d} m)'\n", (int)log10(s));
        fprintf(gnuplotPipe, "set ylabel 'Probability Density'\n");
        fprintf(gnuplotPipe, "set yrange [0:200000]\n");
        fprintf(gnuplotPipe, "set output '%s'\n", outfile);
        fprintf(gnuplotPipe,
"plot \"%s\" using 1:2 w l ls 1 title 'True', \"%s\" using 1:3 w l ls 3 title 'Estimate'\n",
        dtfile, dtfile);
        fprintf(gnuplotPipe, "set label '%0.6fs' at -150,3.5 center textcolor lt 1\n",
(float)x * dt);
        fprintf(gnuplotPipe, "set yrange [-10:10]\n");
        fprintf(gnuplotPipe, "set ylabel 'Phase (rad)'\n");
        fprintf(gnuplotPipe, "set output '%s'\n", outfile1);
        fprintf(gnuplotPipe,
"plot \"%s\" using 1:2 w l ls 1 title 'True', \"%s\" using 1:3 w l ls 3 title 'Estimate'\n",
        dtfile1, dtfile1);
        fflush(gnuplotPipe);
        fclose(gnuplotPipe);
    }
}
/*=====*/
}

void plot_data()
{
    /*=====*/
    /* Declare variables */
    /*=====*/
    FILE *gnuplotPipe;
    /*=====*/
    /* Open pipe, plot data using Gnuplot and close */
    /*=====*/
    printf("Plotting quantitative data...\n");
    gnuplotPipe = popen("gnuplot -persist", "w");
    if (gnuplotPipe)
    {
        fprintf(gnuplotPipe, "cd 'quantitative'\n");
        fprintf(gnuplotPipe, "load \"plot.p\"\n");
        fflush(gnuplotPipe);
    }
    fclose(gnuplotPipe);
    /*=====*/
}

void make_movie()
{
    /*=====*/
    /* Make movies using ffmpeg */
    /*=====*/
    //system("ffmpeg -r 10 -i wavefunction/%06d.jpeg wavefunction.mp4");
}

```

```

//system("ffmpeg -r 10 -i phase/%06d.jpeg phase.mp4");
system("ffmpeg -r 10 -i wavefunction/%06d.jpeg wavefunction.avi");
system("ffmpeg -r 10 -i phase/%06d.jpeg phase.avi");
/*****
}

```

record_initial.c

```

/*
COMMENT: This file contains the function that records the
        initial wave functions and phases to data files...
*/
#include "constants.h"
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <complex.h>
#include <omp.h>

void record_initial(_Complex double phi[], _Complex double phie[])
{
    /*****
    /* Declare and initialize variables */
    /*****
    FILE *fp, *fpl, *fs;
    int x, flag = 0, flag1 = 0;
    /*****
    /* Open data files, record data and close */
    /*****
    fp = fopen("wavefunction/data000000.dat", "wb");
    fpl = fopen("phase/data000000.dat", "wb");
    for(x = xglo; x <= xgup; x += xres)
    {
        fprintf(fp, "%d\t%f\t%f\n", x,
            cabs(phi[(x - xlower) / xres]) * cabs(phi[(x - xlower) / xres]),
            cabs(phie[(x - xlower) / xres]) * cabs(phie[(x - xlower) / xres]));
        if(cabs(phi[(x - xlower) / xres]) < 1e-3 && cabs(phie[(x - xlower) / xres]) < 1e-3)
            fprintf(fpl, "%d\t%f\t%f\n", x, 0.0, 0.0);
        else if(cabs(phi[(x - xlower) / xres]) < 1e-3 && cabs(phie[(x - xlower) / xres]) > 1e-3)
            fprintf(fpl, "%d\t%f\t%f\n", x, 0.0,
                fmod(carg(phie[(x - xlower) / xres]) / cabs(phie[(x - xlower) / xres]), 2 * PI));
        else if(cabs(phi[(x - xlower) / xres]) > 1e-3 && cabs(phie[(x - xlower) / xres]) < 1e-3)
            fprintf(fpl, "%d\t%f\t%f\n", x,
                fmod(carg(phi[(x - xlower) / xres]) / cabs(phi[(x - xlower) / xres]), 2 * PI), 0.0);
        else
            fprintf(fpl, "%d\t%f\t%f\n", x,
                fmod(carg(phi[(x - xlower) / xres]) / cabs(phi[(x - xlower) / xres]), 2 * PI),
                fmod(carg(phie[(x - xlower) / xres]) / cabs(phie[(x - xlower) / xres]), 2 * PI));
    }
    fclose(fp);
    fclose(fpl);
    /*****
}

```

record_quant.c

```

/*
COMMENT: This file contains the function that records plot data...
*/
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <complex.h>
#include <time.h>
#include "constants.h"
void frecord1(int timestep, double xbar, double xbare, double fidelity, double varx,
              double varxe, double devx, double devxe, double mx)
{
    /*=====*/
    /* Declare variables */
    /*=====*/
    FILE *p1, *p2, *p3, *p4, *p5, *p6, *p7, *p8;
    /*=====*/
    /* Open data files, record data and close */
    /*=====*/
    p1=fopen("quantitative/mean.dat","a");
    p2=fopen("quantitative/mean1.dat","a");
    p3=fopen("quantitative/fidelity.dat","a");
    p4=fopen("quantitative/variance.dat","a");
    p5=fopen("quantitative/variance1.dat","a");
    p6=fopen("quantitative/stddev.dat","a");
    p7=fopen("quantitative/stddev1.dat","a");
    p8=fopen("quantitative/results.dat","a");
    fprintf(p1, "%e\t%e\n", timestep * dt, xbar);
    fprintf(p2, "%e\t%e\n", timestep * dt, xbare);
    fprintf(p3, "%e\t%e\n", timestep * dt, fidelity);
    fprintf(p4, "%e\t%e\n", timestep * dt, varx);
    fprintf(p5, "%e\t%e\n", timestep * dt, varxe);
    fprintf(p6, "%e\t%e\n", timestep * dt, devx);
    fprintf(p7, "%e\t%e\n", timestep * dt, devxe);
    fprintf(p8, "%e\t%e\n", timestep * dt, mx);
    fclose(p1);
    fclose(p2);
    fclose(p3);
    fclose(p4);
    fclose(p5);
    fclose(p6);
    fclose(p7);
    fclose(p8);
    /*=====*/
}

```

Makefile

```

#
#Makefile:
#
OBJ = main.o calc_quantities.o record.o plots_and_movies.o initialize.o
record_initial.o term_fmt.o second_order_weak.o calc_norm_t.o
ran1.o gasdev.o create_files.o record_quant.o graphics.o

```

```
CC = gcc
CFLAGS = -lm -lncurses
OUT = main
$(OUT): $(OBJ)
$(CC) $(OBJ) -o $(OUT) $(CFLAGS)

clean:
rm -f *.o; rm -f *.dat; rm -f phase/*.dat;
    rm -f wavefunction/*.dat; rm -f phase/*.jpeg;
    rm -f wavefunction/*.jpeg; rm -f *.mpeg
```